Entanglement scaling in Bethe Ansatz solvable models exhibiting quantum phase transitions

Daniel Larsson
danlar@student.chalmers.se

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This result is too beautiful to be false; it is more important to have beauty in one's equations than to have them fit experiment.

P.Dirac

Abstract

The first part of this thesis is devoted to the definition of entanglement in fermionic systems and the derivation of necessary conditions for the calculation of entanglement analytically in the thermodynamic limit. We then introduce the Bethe Ansatz which is used to calculate the ground state energy in the one-dimensional Hubbard model exactly. We also introduce methods to calculate the ground state energy in limits where the Bethe Ansatz equations cannot be solved on closed form. The ground state energy is then used to derive exact expressions for the local entanglement entropy E_ν in the ground state of the one-dimensional Hubbard model at a quantum phase transition driven by a change of on-site interaction U, magnetic field h, or chemical potential μ. For the two latter cases we find that the QPT is associated with a divergence in the first derivative of the local entanglement with respect to the scaling field. The leading divergences of $\partial E_\nu/\partial h$ and $\partial E_\nu/\partial \mu$ are shown to be directly related to those of the zero-temperature spin and charge susceptibilities. Logarithmic corrections to scaling signal a change in the number of local states accessible to the system as it undergoes the transition.

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Chapter 1

Introduction

Quantum entanglement is truly in the heart of quantum mechanics. Much of it's attention started in 1935 when A. Einstein, B. Podolsky and N. Rosen formulated the famous EPR paradox [1] where they argue that quantum mechanics cannot be considered complete since it allows for non local correlations, which by Einstein was termed a "spooky action at a distance" and which we today call *quantum entanglement*. Much of the EPR criticism of quantum mechanics can be easily illustrated by an example proposed by D. Bohm [2]. Consider that we have a spinless system that decays into two spin-1/2 particles, such as $\pi^0 \rightarrow e^+ + e^-$. After the decay the two particles are very far apart and cannot interact. If we now measure the spin component in the x direction of the electron and obtain the result spin up we know with certainty (by spin conservation) that the positron has spin down along the same x-direction. Common sense would tell us that it had to have been in that state from the very instant it was free, since it did not interact with any particle. Quantum mechanics states something else, namely that the spin of the positron was in a linear combination of up and down until we measure the electron. Then the positron immediately attains spin down although there is no interaction between the electron and the positron. Today we know via experimental tests of the Bell inequalities [3] that quantum mechanics is right. For a more comprehensive introduction we recommend [4].

Much of the recent attention on quantum entanglement has two reasons. One is that it can be used as a resource in quantum information theory [5]. The second reason is that there are several conjectures about a connection to quantum phase transitions (QPT) and that it may be the thing that drives the transition. A quantum phase transition is a change in the ground state that is caused solely by quantum fluctuations (instead of thermal fluctuations, as is the case in classical transitions). In this thesis we will focus our attention on the QPT connection and study how entanglement behaves at critical points in the Hubbard model.

Chapter 2

Basic concepts

2.1 Entanglement

To be able to talk about entanglement we have to have a composite system of at least two parts. If we take a system that consists of one proton and one electron we can write the total system as a direct product of the two parts, i.e. $w = u \otimes v$. Let us assume that all composite systems do not differ in any essential way from this elementary case, and in particular we assume that they obey the principle of super position. If u_1, u_2 are possible states for the proton and v_1, v_2 are possible states for the electron we have that

$$w = \alpha v_1 \otimes u_1 + \beta v_2 \otimes u_2 \tag{2.1}$$

is a realizable state of our system. Note that neither the electron nor the proton we have is in a pure quantum state. There is no complete test for the electron or the proton whose result is predictable with certainty. Only the combined system has a well defined pure quantum state, in which the proton and the electron are correlated. This is why we call our state w entangled.

2.2 Quantum phase transitions

A quantum phase transition (QPT) is a phase transition that occurs at zero temperature. This means that temperature cannot drive the QPT, in contrast to classical phase transitions. Instead QPTs are driven by a coupling constant or an external perturbation and in this thesis the focus will be on phase transitions that are driven by a magnetic field or a chemical potential.
In [6] a QPT is defined as a non-analyticity in the ground state energy. This can be created by a level-crossing or an avoided level crossing. A level crossing occurs when we have a dimensionless coupling constant that only couples to a conserved quantity i.e. $H = H_0 + gH_1$ where H_0 and H_1 commute. This means that H_0 and H_1 can be simultaneously diagonalized and that the eigenfunctions are independent of g even though the eigenvalues vary with g. Now an excited state can become the ground-state at a critical coupling strength $g = g_c$ and this creates the nonanlyticity of the ground state energy. A specific example of a level crossing will be discussed in connection with the attractive Hubbard model in sect. (4.3).

2.3 Entanglement vs QPT

Today there exists many results that indicate a connection between QPTs and entanglement [7, 8, 9]. The main inspiration for the work in this thesis is the conjecture proposed by Wu et al. in [8]. In this conjecture it is proposed that one can find a connection between first and second order QPTs and the entanglement measure concurrence (this measure will be defined together with several others in sect. (2.7)). The original definition of a first (second) order QPT is that there is a divergence in the first (second) derivative of the ground state energy. In the Wu et al. conjecture we have that a first (second) order QPT corresponds to a discontinuity (divergence) in the (the first derivative of the) ground state concurrence. Concurrence have so far not been defined for fermionic systems so much of the work in this thesis will be related to this conjecture and the question whether a similar classification can be extended to fermionic systems (using the measure von Neumann entropy).

2.4 Entanglement in fermionic systems

In the definition of entanglement we rely on the product nature of the state space of a composite system. But since we are dealing with fermions our state space is constrained to the antisymmetric subspace of our N-fold tensor product space. In the first part of this section we will discuss why this is the case and in the second part we will discuss if this constitutes a problem. A quantum system can have subsystems that are physically indistinguishable, i.e. if we put a label on each subsystem and perform a test and the result will be the same if we relabel all the subsystems. This implies that statements as "the position of the 'first' particle" will be meaningless. This also has the effect that not all pure states are realizable. Suppose that we have two identical particles and a complete set of orthogonal single-particle states $\{u_n\}$ and $\{v_n\}$, respectively, for the two particles. Which states are possible for the composite system of the two particles? $u_m \otimes v_n$ is only possible if $m = n$ because if $m \neq n$ then $u_m \otimes v_n$ and $u_n \otimes v_m$ are different. This is not allowed since the second state is obtained only by relabeling the two particles. For indistinguishable systems we have the following possible situations:

$$u_m \otimes v_n \qquad m = n \tag{2.2}$$

$$\frac{1}{\sqrt{2}}\left(u_m \otimes v_n + u_n \otimes v_m\right) \qquad m \neq n \tag{2.3}$$

$$\frac{1}{\sqrt{2}}\left(u_m \otimes v_n - u_n \otimes v_m\right) \qquad m \neq n. \tag{2.4}$$

We now run into problem with the super position principle since

$$u_m \otimes v_n = \frac{1}{2}\left(u_m \otimes v_n + u_n \otimes v_m + u_m \otimes v_n - u_n \otimes v_m\right) \qquad m \neq n. \tag{2.5}$$

This problems implies that we can only have state vectors of two particles that are either totally symmetric or antisymmetric (The situation is actually, a bit more complicated. In two spatial dimensions the two state vectors of two particles can have other symmetries, leading to the concept of fractional statistics and anyons [10]). The symmetric particles are the boson and the antisymmetric ones are our fermions. This implies that we will be forced to stay in the antisymmetric part of the Hilbert space. So for our fermionic system we only

have two possibilities

$$u_m \otimes v_m \qquad m = n \tag{2.6}$$

$$\frac{1}{\sqrt{2}}\left(u_m \otimes v_n - u_n \otimes v_m\right) \qquad m \neq n. \tag{2.7}$$

The observant reader has seen that two particles of the same kind are always entangled. This means that if we have a particle in our laboratory it will be affected by the mere presence of another identical particle somewhere else in the universe. Luckily for us this effect is not a matter of concern, for a proof see [4].

When we talk about entanglement we have to have a partition into good subsystems. In the Hubbard model we can choose the lattice points as subsystems. The reason that this choice is a good subsystem is that their occupation numbers are physical observables and do not depend on the particles themselves: We only make a statement that there is a particle with spin up at a given site but we don't say anything about which particle it is. This definition of our subsystem has the interesting effect that we can allow one-particle entanglement, since the one-particle state $|0\rangle\otimes|\uparrow\rangle + |\uparrow\rangle\otimes|0\rangle$ is entangled with the empty state. This seems rather strange but it has been shown that it is in fact possible to use one particle entanglement in quantum teleportation [11].

2.5 The Bell states

Before we start to define different measures of entanglement we start by defining a unit of entanglement. In quantum information theory one often talks about "e-bits" as units of entanglement. An "e-bit" is defined as the amount of entanglement in a maximally entangled state of two qubits or any other pure bipartite state, for which $E_\nu = 1$. The Bell states are examples of quantum states that contain one "e-bit" of entanglement. The Bell states are:

$$|\phi^+\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle|\uparrow\rangle + |\downarrow\rangle|\downarrow\rangle\right) \tag{2.8}$$

$$|\phi^-\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle|\uparrow\rangle - |\downarrow\rangle|\downarrow\rangle\right) \tag{2.9}$$

$$|\psi^+\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle|\downarrow\rangle + |\downarrow\rangle|\uparrow\rangle\right) \tag{2.10}$$

$$|\psi^-\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle\right). \tag{2.11}$$

These states are often referred to as "singlets". If we introduce other phases of the Bell states we obtain the "magic basis":

$$\begin{aligned}
|e_1\rangle &= \frac{1}{\sqrt{2}}\left(|\uparrow\rangle|\uparrow\rangle + |\downarrow\rangle|\downarrow\rangle\right) \\
|e_2\rangle &= \frac{i}{\sqrt{2}}\left(|\uparrow\rangle|\uparrow\rangle - |\downarrow\rangle|\downarrow\rangle\right) \\
|e_3\rangle &= \frac{i}{\sqrt{2}}\left(|\uparrow\rangle|\downarrow\rangle + |\downarrow\rangle|\uparrow\rangle\right) \\
|e_4\rangle &= \frac{1}{\sqrt{2}}\left(|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle\right).
\end{aligned} \tag{2.12}$$

This basis will be used in the definition of entanglement measures in sect. (2.7).

2.6 Von Neumann entropy

The von Neumann entropy [5, 12] is a measure of entanglement which is the quantum version of the classical Shannon entropy. To calculate it we need do two things: divide our system into two parts A (Alice) and B (Bob) and calculate the density matrix of our total system $\rho = |\psi\rangle\langle\psi|$. When this is done we calculate the reduced density matrix which is a reduction of our total density matrix by tracing out Bobs degrees of freedom. If we trace out Bobs degrees of freedom the reduced density matrix is defined as

$$\rho_{H_A} = tr_{H_B}(\rho) = \sum_{|\phi\rangle,|\phi'\rangle\in\mathcal{B}_{H_A}} |\phi\rangle \left(\sum_{|\psi\rangle\in\mathcal{B}_{H_B}} \langle\phi,\psi|\rho|\phi',\psi\rangle \right) \langle\phi'|. \tag{2.13}$$

Here H_A and H_B are the the Hilbert spaces for Alice's and Bob's sites, respectively. $\mathcal{B}_{H_A}$ and $\mathcal{B}_{H_B}$ are the corresponding bases that span Hilbert space H_A and H_B, respectively. We can now define the von Neumann entropy,

$$S(\rho) = -tr(\rho \log_2 \rho). \tag{2.14}$$

When we measure how entangled A is with B we take the von Neumann entropy of the reduced density matrix:

$$E_\nu \equiv S(\rho_A) = S(\rho_B). \tag{2.15}$$

If the density matrix is diagonal in the given basis we see that is reduces to the classical Shannon entropy,

$$S(p) = \sum_{i=1}^{n} p_i \log_2 p_i \quad \text{where} \quad p = (p_1, \cdots, p_n). \tag{2.16}$$

Example

Let's calculate the von Neumann entropy for the pure state

$$|\psi\rangle = \cos(\theta)|\uparrow\rangle_A|\downarrow\rangle_B + \sin(\theta)|\downarrow\rangle_A|\uparrow\rangle_B. \tag{2.17}$$

As we have seen, if we have a physical system composed of two parts A and B that is described by a density matrix ρ, the reduced density matrix operator for subsystem A is defined as

$$\rho_A = tr_B(\rho). \tag{2.18}$$

tr_B is defined by

$$tr_B(|a_1\rangle\langle a_2| \otimes |b_1\rangle\langle b_2|) = |a_1\rangle\langle a_2| tr(|b_1\rangle\langle b_2|). \tag{2.19}$$

Our reduced density matrix is now given by

$$\begin{aligned} \rho_A &= tr_B(\rho) = \cos^2(\theta)|\uparrow\rangle\langle\uparrow|\langle\downarrow|\downarrow\rangle + \sin^2(\theta)|\downarrow\rangle\langle\downarrow|\langle\uparrow|\uparrow\rangle \\ &+ \sin(\theta)\cos(\theta)(|\uparrow\rangle\langle\downarrow|\langle\downarrow|\uparrow\rangle + |\downarrow\rangle\langle\uparrow|\langle\uparrow|\downarrow\rangle) \\ &= \begin{pmatrix} \cos^2(\theta) & 0 \\ 0 & \sin^2(\theta) \end{pmatrix}. \end{aligned} \tag{2.20}$$

With the same calculation we can verify that ρ_B is given by

$$\rho_B = \begin{pmatrix} \sin^2(\theta) & 0 \\ 0 & \cos^2(\theta) \end{pmatrix}. \tag{2.21}$$

The von Neumann entropy is now given by

$$E(\rho_A) = -tr(\rho_A \log_2 \rho_A) = -2(\cos^2(\theta)\log_2(\cos(\theta)) - \sin^2(\theta)\log_2(\sin(\theta))). \tag{2.22}$$

2.7 Other measures of entanglement

Today there exist many different entanglement measures, the von Neumann entropy discussed in sect. (2.6) being one of them. Of the other measures most of them are pairwise ("bipartite") entanglement measures: they measure how much entanglement there is between two spins in a system. Note that all these measures (except the von Neumann entropy) are defined for two-level qubit systems and their generalization to fermionic systems is still an open question. In the rest of this section we will focus our attention on the concurrence measures, with the others measures only being briefly introduced. For a more comprehensive treatment we recommend [13, 14, 15, 16].

2.7.1 Entanglement of formation

Entanglement of formation [14] measures how many maximally entangled states that are needed to construct a given state using a specific set of rules.

2.7.2 Entanglement of assistance

Entanglement of assistance [15] is an opposite extreme of entanglement of formation it is quantified as the number of maximally entangled states that can be extracted from a given state using any types of measurements on the rest of the system.

2.7.3 Localizable entanglement

Localizable entanglement [16] is similar to entanglement of assistance but only allowing local measurements on the spins in the rest of the system.

2.7.4 Concurrence

The concurrence is dual to some entanglement measure. There are different concurrence measures corresponding to different entanglement measures. Since the relation between the entanglement measures and concurrence is bijective it is reasonable to talk about concurrence as an entanglement measure. We will focus on the concurrence of formation and the von Neumann concurrence.

The von Neumann concurrence

For a pure bipartite state $|\psi\rangle = \sum_i a_i |e_i\rangle$ expressed in the "magic basis" in eqn. (2.12) the von Neumann entropy can be written as

$$E_\nu = f(C(\psi)) \tag{2.23}$$

where

$$f(C) \quad = \quad H\left(\frac{1}{2}+\frac{1}{2}\sqrt{1-C2}\right). \tag{2.24}$$

Here H is the binary entropy function

$$H(x) = -x\log_2 x - (1-x)\log_2(1-x) \tag{2.25}$$

and C is the von Neumann concurrence, defined [17] by

$$C(\psi) = \left|\sum_i a_i^2\right|. \tag{2.26}$$

Concurrence of formation

The set of matrices that are real when expressed in the magic basis eqn. (2.12) is the same as the set of density matrices describing mixtures of Bell states. This allows us to form the matrix $R = \sqrt{\sqrt{\rho}\rho^*\sqrt{\rho}}$. tr$R$ ranges from 0 to 1 and is a measure of the degree of equality between ρ and ρ^*, see [17, 18] therein. Since ρ is real for a mixture of Bell states the difference between ρ and ρ^* makes tr$R$ a measure of entanglement. The concurrence of formation is defined as:

$$C_F = max\{0, 2\lambda_{max} - \mathrm{tr}R\} \tag{2.27}$$

where λ_{max} is the largest eigenvalue of R. We can now obtain the entanglement of formation by the simple relation

$$E_F(\rho) = f(C_F) \tag{2.28}$$

where f is given i eqn. (2.24). For a proof of this relation see [17, 19].

2.8 Why von Neumann?

It is now time to discuss why the von Neumann entropy is a natural entanglement measure for a pure state. First of all it has three important properties that we require of a entanglement measure. For a complete list of its properties, see [12]
(1) The entanglement of independent systems are additive. This means that if we have a situation where Alice and Bob share n singlets they have n ebits of entanglement between them.
(2) The von Neumann entropy E_ν is preserved under local unitary operations. This means that any unitary operation that can be written as $U = U_A \otimes U_B$ will preserve the amount of entanglement and this implies that we can not create entangled states from unentangled states through local unitary operations.
(3) The expectation of E_ν cannot be increased by local non-unitary operations i.e. a measurement by Alice or Bob.

But the most important reason why the von Neumann entropy is a natural measure is that we can dilute and concentrate entanglement with unit asymptotic efficiency [14]. This means

that if Alice and Bob is given a supply of n identical qubits in a state $\Psi = (\psi)^n$ they can use local operations and classical one-way communication to prepare m identical maximally entangled qubits in a state $\Phi \approx (\phi)^m$, with the yield m/n approaching $E_\nu(\psi)/E_\nu(\phi)$, the fidelity $|\langle\Phi|(\phi)^m\rangle|$ approaching 1, and the probability of failure approaching zero in the limit of large n. This means that if we let ψ be a Bell state we obtain the asymptotic number of singlets required to locally prepare a system in a given state Φ, its entanglement of formation. If we let ϕ be a Bell state we obtain the number of Bell states that can be extracted from a given system Ψ, its distillable entanglement. Therefore the entanglement is totally parameterized by the von Neumann entropy for a pure bipartite state.

2.9 The Hubbard Hamiltonian

Since we want to study entanglement in a fermionic system, the Hubbard model is a natural choice since it is paradigm for correlated electrons, it is integrable and it possess a number of interesting QPTs. We start by defining the Hamiltonian for the Hubbard model in it's simplest form

$$H = -t\sum_{i=1}^{L}(\hat{c}_{ia}^{\dagger}\hat{c}_{i+1a} + h.c.) + U\sum_{i=1}^{L}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}. \tag{2.29}$$

Here $\hat{c}_{ia}^{\dagger}$ creates a particle at site i with spin component a and $\hat{c}_{ia}$ annihilates a particle at site i with spin component a. The first terms in our Hamiltonian control the jumping between sites since $\hat{c}_{i+1a}$ annihilates a particle with spin component a at site $i+1$ $\hat{c}_{ia}^{\dagger}$ creates an identical particle at site i. In this thesis we will always put t=1 and this can be done without loss of generality. The second term in the Hamiltonian measures how many sites have double occupancy and since we are dealing with fermions the only possible configuration with two particles at one site is one particle with spin up and the other with spin down. When we have $U \to \infty$ there are no double occupancies and when $U \to -\infty$ we have only double occupancies.

2.10 Symmetries and the search for a diagonal density matrix

Since our main interest in this thesis is the Hubbard model it is now time to discuss how we shall measure entanglement in this model [20]. Since we want to calculate entanglement in the thermodynamic limit $N, L \to \infty$ we can not calculate the total density matrix directly by taking the outer product of the ground state $|\psi\rangle$ whit itself i.e. $\rho = |\psi\rangle\langle\psi|$. So let us focus on what we actually *can* calculate. As will be seen later in this thesis we can calculate the occupation number of our four local states $|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle$. Luckily for us, this is sufficient if our reduced density matrix is diagonal in this basis. In this case, with Alice having one site, it attains the following form if we trace away Bob's degrees of freedom:

$$\rho_{\hat{j}} = z|0\rangle\langle 0| + u^{+}|\uparrow\rangle\langle\uparrow| + u^{-}|\downarrow\rangle\langle\downarrow| + \omega|\uparrow\downarrow\rangle\langle\uparrow\downarrow|. \tag{2.30}$$

Here our parameters in the density matrix are given by

$$\omega = \langle\hat{n}_{j\uparrow}\hat{n}_{j\downarrow}\rangle = tr(\hat{n}_{j\uparrow}\hat{n}_{j\downarrow}\rho_j) \tag{2.31}$$

$$u^{+} = \langle\hat{n}_{j\uparrow}\rangle - \langle\hat{n}_{j\uparrow}\hat{n}_{j\downarrow}\rangle \tag{2.32}$$

$$u^{-} = \langle\hat{n}_{j\downarrow}\rangle - \langle\hat{n}_{j\uparrow}\hat{n}_{j\downarrow}\rangle \tag{2.33}$$

$$z = 1 - u^{+} - u^{-} - \omega. \tag{2.34}$$

Let us prove eqn. (2.31)

$$\begin{aligned}\langle \hat{n}_{j\uparrow}\hat{n}_{j\downarrow}\rangle &= tr(\hat{n}_{j\uparrow}\hat{n}_{j\downarrow}\rho_j) \\ &= tr(\hat{n}_{j\uparrow}\hat{n}_{j\downarrow}(z|0\rangle\langle 0| + u^+|\uparrow\rangle\langle\uparrow| + u^-|\downarrow\rangle\langle\downarrow| + \omega|\uparrow\downarrow\rangle\langle\uparrow\downarrow|)) \\ &= tr(\omega|\uparrow\downarrow\rangle\langle\uparrow\downarrow|) = \omega.\end{aligned} \tag{2.35}$$

We can easily see that eqn. (2.32)-eqn. (2.34) will follow by a similar calculation. How do we guarantee that our reduced density matrix is diagonal? To answer this question we start by studying how the off-diagonal elements are created. To create an off-diagonal element we must have a state that is a linear combination of states where Bob's sites have the same occupation numbers and Alice's sites have different occupation numbers. Let us illustrate this by an example.

Example

If we have the following state $|\psi\rangle = |AB\rangle + |A'B\rangle$ the density matrix will have the form

$$\rho = |\psi\rangle\langle\psi| = |AB\rangle\langle AB| + |AB\rangle\langle A'B| + |A'B\rangle\langle AB| + |A'B\rangle\langle A'B|. \tag{2.36}$$

We now see that if $A \neq A'$ then $|AB\rangle\langle A'B|$ and $|A'B\rangle\langle AB|$ will create off-diagonal elements if we trace out Bob's degrees of freedom. If we have different occupation numbers on Bob's sites then the inner product $\langle\phi,\psi|\rho|\phi',\psi\rangle$ will always be zero for the corresponding elements of the density matrix.

If we require that our ground state is a superposition of states with the same number of particles and the same total spin then only superpositions of states with the same eigenvalues of $\sum_{i=1}^{L}(\hat{n}_{i,\uparrow} + \hat{n}_{i,\downarrow})$ and $\sum_{i=1}^{L}(\hat{n}_{i,\uparrow} - \hat{n}_{i,\downarrow})$ are allowed. To get site independence we also require that we have translational invariance. The first two conditions mean that we can not have a superposition of states where Alice's sites are different and Bob's are the same. This is so since if the number of particles and the total spin are the same for all states in our superposition then we can create one from the other by moving around particles. Therefore, if we change Alice's site by removing or adding one particle this particle has to go to or come from somewhere and this "somewhere" are Bob's sites. To summarize, we note that in every superposition of states where Alice's site are different at least one of Bob's sites has to be different and the inner product $\langle\phi,\psi|\rho|\phi',\psi\rangle$ in eqn. (2.13) will always be zero for the corresponding elements of the density matrix. We can now give the explicit formula for the von Neumann entropy in the Hubbard model:

$$E_\nu(\rho) = -z\log_2 z - u^+\log_2 u^+ - u^-\log_2 u^- - \omega\log\omega. \tag{2.37}$$

2.11 Hellman-Feynman theorem

The Hellman-Feynman theorem [21] states that

$$\frac{\partial E}{\partial\lambda} = \left\langle \frac{\partial H}{\partial\lambda} \right\rangle. \tag{2.38}$$

The proof is simple:

$$\frac{\partial E}{\partial \lambda} = \frac{\partial}{\partial \lambda}\langle\psi|H|\psi\rangle \tag{2.39}$$

$$= \langle\frac{\partial \psi}{\partial \lambda}|H|\psi\rangle + \langle\psi|\frac{\partial H}{\partial \lambda}|\psi\rangle + \langle\psi|H|\frac{\partial \psi}{\partial \lambda}\rangle \tag{2.40}$$

$$= E\frac{\partial}{\partial \lambda}\langle\psi|\psi\rangle + \langle\psi|\frac{\partial H}{\partial \lambda}|\psi\rangle, \tag{2.41}$$

using that H is Hermitian. Since $\langle\psi|\psi\rangle = 1$, assuming that the state $|\psi\rangle$ is normalized, we obtain

$$\frac{\partial E}{\partial \lambda} \equiv \left\langle \frac{\partial H}{\partial \lambda} \right\rangle. \tag{2.42}$$

This result will be very useful for us since if we take the derivative of our Hamiltonian w.r.t. U we will get the double occupancy. This can easily be seen by performing the following calculation

$$\frac{1}{L}\frac{\partial E_0}{\partial U} = \frac{1}{L}\left\langle \frac{\partial H}{\partial U} \right\rangle = \frac{1}{L}\left\langle \sum_{i=1}^{L} \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} \right\rangle = \frac{1}{L}\sum_{i=1}^{L}\langle \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}\rangle = \frac{1}{L}\sum_{i=1}^{L}\omega = \frac{L}{L}\omega = \omega. \tag{2.43}$$

Here we have used that $\langle \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}\rangle$ is site independent since H is invariant under translation. The only thing that is stopping us now from calculating the von Neumann entropy is the question how we calculate the ground state energy in the Hubbard model. We will use the next chapter to answer this question by the use of Bethe's ansatz.

Chapter 3

Bethe's ansatz

In this chapter we will introduce Bethe's ansatz and use it to calculate the ground state energy in the Hubbard model [22, 23, 24, 25, 26]. We then introduce methods for calculating the ground state energy when we can't solve the Bethe Ansatz equations on closed form [24, 27, 28]. As mentioned in the previous section the reason why we want to calculate the ground state energy is that we can use the Hellman-Feynman theorem to calculate the double occupancy, magnetization as a function of the magnetic field and filling as a function of the chemical potential. This we will then use in the subsequent sections to calculate the entanglement.

3.1 Integrable systems

The term *integrable model* originates from classical Hamiltonian mechanics. In classical mechanics a system is integrable if it possesses as many degrees of freedom as it has constants of motion. If we have a classical Hamiltonian $H(p,q)$ with N degrees of freedom where $p = \{p_i\}_{i=1}^N$ and $q = \{q_i\}_{i=1}^N$ are generalized coordinates H is completely integrable if there exist N independent functions $I_i(p,q)$ such that

$$\{H, I_i\} = 0 \quad \{I_i, I_j\} = 0, \quad i = 1, 2, \cdots, N. \tag{3.1}$$

Here $I_i(p,q)$ are our constants of motion. It is now possible to solve the system exactly by transforming to action-angle variables $(p_i, q_i) \to (I_i, \varphi_i)$. In our new coordinates we can write our equations of motion as

$$\dot{I}_i = \{H, I_i\} = 0, \tag{3.2}$$

$$\dot{\varphi}_i = \{H, \varphi_i\} = \omega_i(I_i). \tag{3.3}$$

We now have that

$$I_i = \text{constant} \qquad \varphi_i(t) = \varphi_i(0) + \omega_i t \tag{3.4}$$

is a solution to our system. In this thesis our interest lies in exactly solvable many-body systems in condensed matter physics. For these models the history started in 1931 with H. Bethe's solution of the Heisenberg model [29]. In his work he constructed a many-body wave function and reduced the problem of calculating the spectrum of the Hamiltonian to solving a set of N coupled algebraic equations. At the time Bethe's work was considered

to be a fascinating but mostly an academic exercise. One hoped that it might serve as a first step toward a solution of the Heisenberg model in two and three dimensional lattices. The second milestone was the solution of the two-dimensional Ising model [30] performed by L. Onsager in 1944. In the 1960's things really started to take off and new applications of Bethe's ansatz were discovered. For an overview of the work performed we recommend the first chapter in [25]. It was also in the 1960's that the Hubbard model started it's "career" as an exactly solvable model in a paper [22] by E.H. Lieb and F.Y. Wu published in 1968. These authors succeeded in calculating the ground state energy and demonstrate that the Hubbard model undergoes a Mott metal-insulator transition at half-filling with the critical interaction strength U=0. For an overview of the work on the Hubbard model we again recommend [25]. But now we start our own work with the solution of the Hubbard model.

3.2 The S-matrix for the Hubbard model

Our starting point is the Hamiltonian for the Hubbard model,

$$H = -t\sum_{i=1}^{L}(\hat{c}_{ia}^{\dagger}\hat{c}_{i+1a} + h.c.) + U\sum_{i=1}^{L}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}. \tag{3.5}$$

We shall study this Hamiltonian in a Hilbert space $\mathcal{H}_N$ of N particles, defined with respect to the vacuum state $|0\rangle$ that contains none. This Hilbert space is spanned by states of the form

$$|F\rangle = \sum_{a_1\cdots a_N}\sum_{b_1\cdots b_N} F_{a_1\cdots a_N}(n_1\cdots n_N)\prod_{i=1}^{N}\hat{c}_{a_i n_i}^{\dagger}|0\rangle. \tag{3.6}$$

We next introduce the most important equation in Physics, the Schrödinger equation:

$$H|F\rangle = E|F\rangle. \tag{3.7}$$

We have written the equation in a second-quantization description since the Hamiltonian in eqn. (3.5) is second quantized. We now want to pass to a first quantization description. To do this we start by replacing the jump terms $\hat{c}_{i+1a}^{\dagger}\hat{c}_{ia}$ by a hopping operator Δ_j given by:

$$\Delta_j F_{a_1\cdots a_N}(n_1\cdots n_N) = F_{a_1\cdots a_N}(n_1\cdots n_j+1\cdots n_N) + F_{a_1\cdots a_N}(n_1\cdots n_j-1\cdots n_N). \tag{3.8}$$

From now on F is the amplitude of a given wave function. The operator $\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$ can be replaced by a delta function and the first quantized version of the Hamiltonian attains the form

$$h = -t\sum_{j=1}^{N}\Delta_j + U\sum_{j<l}\delta_{n_j n_l}. \tag{3.9}$$

We can reformulate eqn. (3.7) by using eqn. (3.9)

$$hF = EF. \tag{3.10}$$

It is now time to diagonalize h within $\mathcal{H}_N$. We start from the wave function. Since we are dealing with fermions it is antisymmetric and it is given by

$$\begin{aligned} F_{a_1a_2}(n_1,n_2) &= e^{ik_1n_1+ik_2n_2}[A_{a_1a_2}\theta(n_1-n_2) + B_{a_1a_2}\theta(n_2-n_1)] \\ &- e^{ik_1n_2+ik_2n_1}[A_{a_2a_1}\theta(n_2-n_1) + B_{a_2a_1}\theta(n_1-n_2)]. \end{aligned} \tag{3.11}$$

Here θ is the step function defined by

$$\theta(x) = \begin{cases} 0, & x < 0 \\ 1/2, & x = 0 \\ 1, & 0 < x \end{cases} . \tag{3.12}$$

The cautious reader may verify that $F_{a_1 a_2}(n_1, n_2)$ in eqn. (3.11) is a solution by inserting it into eqn. (3.10). By this computation one also realizes that

$$E = -2t(\cos k_1 + \cos k_2). \tag{3.13}$$

Let us continue by defining the S-matrix which relates the A and B amplitudes:

$$B_{a_1 a_2} = S^{b_1 b_2}_{a_1 a_2} A_{b_1 b_2}. \tag{3.14}$$

The first step in the diagonalization process is to find a explicit form for this S-matrix by using some of the properties of the wave function F. Our wave function $F(n, n)$ has to be defined independently of region because of it's fermionic nature. This condition can be formulated in terms of our amplitudes A and B as

$$A_{a_1 a_2} - B_{a_2 a_1} = B_{a_1 a_2} - A_{a_2 a_1}. \tag{3.15}$$

This expression can be rewritten by using the spin exchange operator P (with components $P^{b_1 b_2}_{a_1 a_2} = \delta^{b_2}_{a_1} \delta^{b_1}_{a_2}$ and the identity operator, and writing the two sides of eqn. (3.15) in terms of the A amplitude only:

$$A_{a_1 a_2} - B_{a_2 a_1} = (I - PS) A_{b_1 b_2} \tag{3.16}$$

$$B_{a_1 a_2} - A_{a_2 a_1} = (S - P) A_{b_1 b_2}. \tag{3.17}$$

We can now rewrite eqn. (3.15) as

$$I - PS = S - P. \tag{3.18}$$

By shuffling around the terms and multiplying both sides by $\frac{1}{4}(I + P)$ we get

$$\frac{1}{4}(I + P)(I + P) = \frac{1}{4}(I + P)S(I + P). \tag{3.19}$$

This can be rewritten by using $P^2 = I$:

$$\frac{1}{2}(I + P)S\frac{1}{2}(I + P) = \frac{1}{2}(I + P). \tag{3.20}$$

We can verify that if the S-matrix takes the form

$$S = \frac{1}{2}(I + P) + \frac{1}{2}(I - P)s, \tag{3.21}$$

where s is a scalar function, it will fulfill eqn. (3.20). In the final step, to get an explicit form of S, we have to calculate s. To do this we use the Schrödinger equation (3.10) and our Ansatz for the wave function eqn. (3.11). We also use our operators I,P and S to get a wave function that only depends on the amplitude A. The Schrödinger equation for $F(n, n)$ is given by

$$-t[F(n+1, n) + F(n-1, n) + F(n, n+1) + F(n, n-1)] + UF(n, n) = EF(n, n). \tag{3.22}$$

This is equivalent to

$$\begin{aligned} & e^{i(k_1+k_2)n}[(-t)((e^{ik_1}+e^{-ik_2})s+e^{-ik_1}+e^{ik_2})+U\tfrac{1+s}{2}](I-P)A \\ & = -2t(\cos k_1+\cos k_2)e^{i(k_1+k_2)n}\tfrac{1+s}{2}(I-P)A. \end{aligned} \tag{3.23}$$

Now we are almost done. What remains is to solve for s and put this into eqn. (3.21) and we obtain our explicit expression for S, given by

$$S^{jl} \equiv S^{b_j b_l}_{a_j a_l} = \frac{(\sin k_j - \sin k_l)I^{jl} + i\frac{u}{2}P^{jl}}{(\sin k_j - \sin k_l) + i\frac{u}{2}}. \tag{3.24}$$

3.3 The generalization to N particles and the Yang-Baxter equation

So far we have only studied the two-particle case and it's time to generalize our result to N particles. In the N-particle case we use the notation S^{ij} for simplicity to indicate that the S-matrix operates on all N particles but only non-trivially on particle i and j. When we have N particles we have to start dividing the configuration space into $N!$ regions. We label our region $Q = (Q_1, Q_2, \cdots, Q_N)$. We now define the Bethe form of the wave function as

$$F_{a_1 \cdots a_N}(n_1 \cdots n_N) = \mathcal{A} e^{i\sum_j k_j n_j} \sum_Q A_{a_1 \cdots a_N}(Q)\theta(n_Q). \tag{3.25}$$

From the two-particle case, eqn. (3.13), we know that the ground state energy for two particles are given by $E = -2t(\cos k_1 + \cos k_2)$. A straightforward generalization gives that the ground state energy for N particles is given by

$$E = -\sum_j 2t\cos k_j. \tag{3.26}$$

The momentum is given by

$$P = \sum_j k_j. \tag{3.27}$$

How are the amplitudes of different regions Q, Q' related? If they are adjacent, i.e. Q differing from Q' by a single transposition, then they are related by

$$A_{a_1 \cdots a_j \cdots a_l \cdots a_N}(Q') = (S^{jl})^{b_1 \cdots b_N}_{a_1 \cdots a_N} A_{b_1 \cdots b_N}(Q) = (S^{jl})^{b_j b_l}_{a_j a_l} A_{a_1 \cdots b_j \cdots b_l \cdots a_N}(Q). \tag{3.28}$$

When this is not the case we can always find a path that relates Q with Q'. If for example

$$Q = P^{ij}P^{jk}P^{kl}Q' \tag{3.29}$$

then

$$A(Q) = S^{ij}S^{jk}S^{kl}A(Q'). \tag{3.30}$$

In most cases we can find more than one path, the simplest example is if we have three particles. We then have three ways to collide the particles which are illustrated in figs. (3.1) and (3.2). Since we want that the result should be path-independent we need these three pictures to be equivalent, i.e. that each many-body collision can be viewed as a sequence

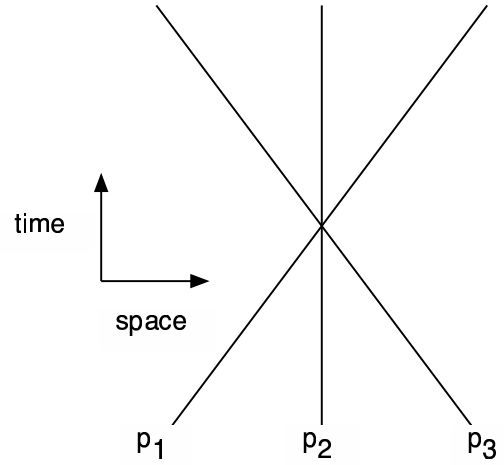


Figure 3.1: The three body scattering S^{123}

of independent two-body collisions. This last statement can be reformulated in terms of our S-matrices as

$$S^{123} = S^{12}S^{13}S^{23} = S^{23}S^{13}S^{12}. \tag{3.31}$$

This is the famous Yang-Baxter equation (YBE) [31]. Considerations in the case $N = 2$ and $N = 4$ also require that two more conditions are fulfilled in order to guarantee path independence for all N. These are:

$$\begin{aligned} S^{ij}S^{ji} &= I \\ S^{ij}S^{kl} &= S^{kl}S^{ij}. \end{aligned} \tag{3.32}$$

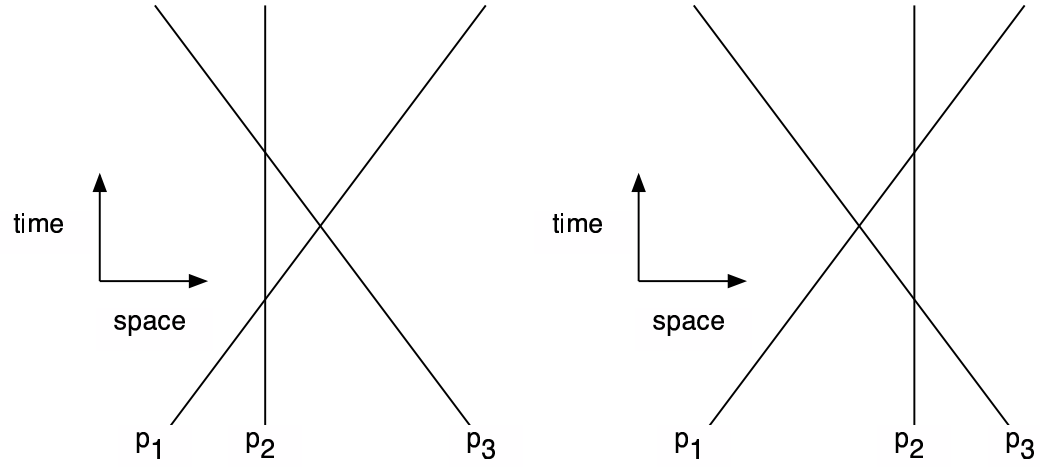
The YBE is one of the most important equations that we will introduce in this thesis since if an S-matrix fulfills it, then the corresponding Hamiltonian will be integrable. We are now in a position such that we can reformulate the Bethe form, eqn. (3.25), of the wave function:

$$F_{a_1\cdots a_N}(n_1\cdots n_N) = \mathcal{A}e^{i\sum_j k_j n_j}\sum_Q S(Q)A_{a_1\cdots a_N}(I)\theta(n_Q). \tag{3.33}$$

In this new version of the Bethe form we have defined a reference region I, with $A_{a_1\cdots_N}$ the corresponding amplitude for this region. By using our P operator repeatedly on I we can find a path to reach every possible particle configuration. These actions with P on I correspond to actions with S on A as defined in eqn. (3.30). S(Q) is the corresponding product of S-matrices and $\mathcal{A}$ is the usual antisymmetrizer. We will now study a model on a finite ring with length L. With a ring we impose periodic boundary conditions

$$F(\cdots n_j = 0\cdots) = F(\cdots n_j = L\cdots). \tag{3.34}$$

What will this condition mean for the the wave function in a single region? We start from an amplitude $A_{a_1\cdots a_N}(Q)$ and then we act on it with our operator S^{jj+1} to exchange particle j with particle j+1 to it's right. We then do the same with particle j+2 which is to the right of particle j after the previous exchange. We continue this way until we reach the right end of the system. By starting from the same amplitude but instead of moving particle j to the



(a) The two body scattering $S^{23}S^{13}S^{12}$ (b) The two body scattering $S^{12}S^{13}S^{23}$

Figure 3.2: Two body scattering processes

right we move it to the left with the operators S^{j-1j} and so on until we reach the left end of our system. In this way we will get the following relation between our modified amplitudes, given by eqns. (3.34) and (3.33):

$$S^{1j}\cdots S^{j-1j}A(Q) = S^{jN}\cdots S^{jj+1}A(Q)e^{ik_jL}. \tag{3.35}$$

If we now multiply both sides in eqn. (3.35) from the left with $S^{jj-1}\cdots S^{j1}$ and use eqn. (3.32) we obtain

$$A(Q) = S^{j1}\cdots S^{jj-1}S^{jN}\cdots S^{jj+1}e^{ik_jL}A(Q). \tag{3.36}$$

Introducing a new operator

$$Z_j = S^{j1}\cdots S^{jj-1}S^{jN}\cdots S^{jj+1}, \tag{3.37}$$

we can rewrite eqn. (3.36) by dividing both sides by e^{ik_jL} and use our new operator Z_j:

$$Z_jA(Q) = e^{-ik_jL}A(Q). \tag{3.38}$$

This last relation, eqn. (3.38), will be important in the next section when we derive the Bethe-Ansatz equations, since it tells us that e^{-ik_jL} is an eigenvalue to Z_j.

3.4 The Bethe Ansatz equation

In this section we use the Quantum inverse method to derive the Bethe Ansatz equation. Our goal in this section is to find the eigenvectors and eigenvalues of the Z_j operator defined by eqn. (3.37). Here S^{ij} is defined by

$$S^{ij} = \frac{(\alpha_i-\alpha_j)I^{ij}+iUP^{ij}/2}{(\alpha_i-\alpha_j)+iU/2}, \tag{3.39}$$

where $\alpha_j = \sin k_j$. We start by introducing a continuous parameter α into the definition of the S-matrix:

$$S(\alpha) = \frac{\alpha I + iUP/2}{\alpha + iU/2} \equiv a(\alpha)I + b(\alpha)P, \tag{3.40}$$

such that the continuous version of the YBE is fulfilled:

$$S^{kj}(\alpha - \beta)S^{ki}(\alpha)S^{ji}(\beta) = S^{ji}(\beta)S^{ki}(\alpha)S^{kj}(\alpha - \beta). \tag{3.41}$$

Our next step is to introduce an auxiliary spin space V_A and define an S-matrix that acts non-trivially in $V_J \otimes V_A$. It is given by

$$S^{jA}(\alpha) = \frac{\alpha I^{jA} + iUP^{jA}/2}{\alpha + iU/2}. \tag{3.42}$$

The so called *monodromy matrix* is defined by

$$\Xi(\alpha) = \prod_{j=1}^{N} S^{jA}(\alpha - \alpha_j). \tag{3.43}$$

Our next step is to define the trace of Ξ over the auxiliary space $Z(\alpha) = tr_A \Xi(\alpha)$. Z is called the transfer matrix and we will show that for $\alpha = \alpha_j$ we will have $Z = Z_j$ by using $S^{jA}(0) = P^{jA}$. In this proof we will reserve the notation S^{ij} for $S^{ij} = S^{ij}(\alpha_i - \alpha_j)$

$$\begin{aligned} tr_A\Xi(\alpha_j) &= tr_A(S^{1A}(\alpha_j - \alpha_1)\cdots S^{j-1A}(\alpha_j - \alpha_{j-1})P^{jA}S^{j+1A}(\alpha_j - \alpha_{j+1})\cdots S^{NA}(\alpha_j - \alpha_N)) \\ &= tr_A(S^{j+1A}(\alpha_j - \alpha_{j+1})\cdots S^{NA}(\alpha_j - \alpha_N)S^{1A}(\alpha_j - \alpha_1)\cdots S^{j-1A}(\alpha_j - \alpha_{j-1})P^{jA}) \\ &= tr_A(P^{jA}S^{j+1j}(\alpha_j - \alpha_{j+1})\cdots S^{Nj}(\alpha_j - \alpha_N)S^{1j}(\alpha_j - \alpha_1)\cdots S^{j-1j}(\alpha_j - \alpha_{j-1})). \end{aligned} \tag{3.44}$$

We have here used the cyclic property of the trace:

$$tr(XY) = tr(YX), \tag{3.45}$$

and the fact that if we exchange the order of P and S we have the following relation

$$S^{iA}P^{jA} = P^{jA}S^{ij}. \tag{3.46}$$

Now we recall that since our model is integrable we have that $S^{ij}S^{kl} = S^{kl}S^{ij}$ according to eqn. (3.32). Hence we can shuffle around our S-matrices in eqn. (3.44) and obtain:

$$\begin{aligned} tr_A\Xi(\alpha_j) &= tr_A(P^{jA}S^{j-1j}(\alpha_j - \alpha_{j-1})\cdots S^{1j}(\alpha_j - \alpha_1)S^{Nj}(\alpha_j - \alpha_N)\cdots S^{j+1j}(\alpha_j - \alpha_{j+1})) \\ &= tr_A(P^{jA}S^{jj-1}\ldots S^{j1}S^{jN}\ldots S^{jj+1}) \\ &= S^{jj-1}\ldots S^{j1}S^{jN}\ldots S^{jj+1} = Z_j. \end{aligned} \tag{3.47}$$

It is left to show that $S^{ij}(\alpha_j - \alpha_i) = S^{ji}$:

$$\begin{aligned} S^{ij}(\alpha_j - \alpha_i) &= \frac{(\alpha_j - \alpha_i)I^{ij} + iUP^{ij}/2}{\alpha_j - \alpha_i + iU/2} = \\ &= \frac{(\alpha_j - \alpha_i)I^{ji} + iUP^{ji}/2}{\alpha_j - \alpha_i + iU/2} = S^{ji}, \end{aligned} \tag{3.48}$$

using that $I^{ij} = I^{ji}$ and $P^{ij} = P^{ji}$. We can now reformulate our original problem of diagonalizing the Hamiltonian H for the Hubbard model to the problem of diagonalizing our new operator $Z = tr_A \Xi$. A sufficient condition for $Z(\alpha)$ and $Z(\beta)$ to commute is that there exists a matrix R acting in $V_A \otimes V_B$ that fulfills the condition

$$R(\Xi(\alpha) \otimes \Xi(\beta)) = (\Xi(\beta) \otimes \Xi(\alpha))R. \tag{3.49}$$

To prove this we use eqn. (3.45) and note that

$$\Xi(\alpha) \otimes \Xi(\beta) = R^{-1}(\Xi(\beta) \otimes \Xi(\alpha))R. \tag{3.50}$$

By multiplying eqn. (3.49) by R^{-1} we now prove our statement:

$$\begin{aligned} Z(\alpha)Z(\beta) &= tr_{AB}(R^{-1}(\Xi(\beta) \otimes \Xi(\alpha))R) \\ &= tr_{AB}((\Xi(\beta) \otimes \Xi(\alpha))RR^{-1}) \\ &= tr_{AB}(\Xi(\beta) \otimes \Xi(\alpha)) = Z(\beta)Z(\alpha). \end{aligned} \tag{3.51}$$

The reason for our interest in the commutativity of $Z(\alpha)$ and $Z(\beta)$ is that if they commute the system is integrable. We shall now investigate if we can find an R matrix that will fulfill eqn. (3.49). It would be very fortunate if we could find an R-matrix and relate it to the continuous YBE in eqn. (3.41) such that it also guarantees the integrability of our system. We choose our R-matrix in the following way:

$$R = R(\alpha - \beta) = S(\alpha - \beta)P. \tag{3.52}$$

One can show that this choice will fulfill the continuous YBE in eqn. (3.41), implying that $Z(\alpha)$ and $Z(\beta)$ commute. We will now study our problem more explicitly in the auxiliary space. In matrix representation we have:

$$R = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{ic}{\alpha+ic} & \frac{\alpha}{\alpha+ic} & 0 \\ 0 & \frac{\alpha}{\alpha+ic} & \frac{ic}{\alpha+ic} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} a+b & 0 & 0 & 0 \\ 0 & b & a & 0 \\ 0 & a & b & 0 \\ 0 & 0 & 0 & a+b \end{pmatrix}. \tag{3.53}$$

with the monodromy matrix given by

$$\Xi(\alpha) = \begin{pmatrix} A(\alpha) & B(\alpha) \\ C(\alpha) & D(\alpha) \end{pmatrix}. \tag{3.54}$$

Here our operators A,B,C and D operate in the physical space. Eqn. (3.49) can be used to derive some useful algebraic relations, for details, see appendix A. Here we just list a few of the ones most useful for our purpose:

$$\begin{aligned} A(\alpha)B(\beta) &= u(\beta - \alpha)B(\beta)A(\alpha) + v(\beta - \alpha)B(\alpha)A(\beta) \\ D(\alpha)B(\beta) &= u(\alpha - \beta)B(\beta)A(\alpha) + v(\alpha - \beta)B(\alpha)A(\beta) \end{aligned} \tag{3.55}$$

with

$$u(\alpha) = \tfrac{1}{a(\alpha)} = \frac{\alpha + ic}{\alpha} \tag{3.56}$$

$$v(\alpha) = -\tfrac{b(\alpha)}{a(\alpha)} = -\frac{ic}{\alpha}. \tag{3.57}$$

Furthermore

$$[X(\alpha), X(\beta)] = 0, \qquad X = A, B, D. \tag{3.58}$$

We will use these expression to diagonalize $Z(\alpha) = A(\alpha) + D(\alpha)$ and derive the Bethe equations. We start by defining a "reference state" that we take to be the ferromagnetic ground state:

$$|\omega\rangle = \prod_{j=1}^{N} \begin{pmatrix} 1 \\ 0 \end{pmatrix}_j . \tag{3.59}$$

If we act on this state with our operator B it will create eigenstates to our Hamiltonian $A(\alpha) + D(\alpha)$ if we disregard unwanted terms generated by the second term of the right hand side of eqn. (3.55). We will see that we can make these unwanted terms vanish so they will not cause any problem. To see how all this works, let us first show that $|\omega\rangle$ is an eigenstate of our Hamiltonian. For this purpose it is useful to have $S^{jA}(\alpha)$ written explicitly as a matrix:

$$\begin{aligned} S^{jA}(\alpha) &= (a + b/2)(\alpha) I_j I_A + b/2(\alpha)\sigma_j \sigma_A \\ &= (a + b/2)(\alpha) I_j \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\ &+ (b/2)(\alpha) \left(\sigma_j^x \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \sigma_j^y \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + \sigma_j^z \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right) \\ &= \begin{pmatrix} (a + b/2)(\alpha) I_j + (b/2)(\alpha)\sigma_j^z & b(\alpha)\sigma_j^- \\ b(\alpha)\sigma_j^+ & (a + b/2)(\alpha) I_j - (b/2)(\alpha)\sigma_j^z \end{pmatrix}. \end{aligned} \tag{3.60}$$

Here we have used the identity $(P^{jA})^{b,v}_{a,u} = (1/2)(\delta^b_a \delta^v_u + (\sigma_j)^b_a (\sigma_A)^v_u)$. If we now let S^{jA} act on the j^{th} local state in eqn. (3.59), we have

$$S^{jA}(\alpha - \alpha_j) \begin{pmatrix} 1 \\ 0 \end{pmatrix}_j = \begin{pmatrix} 1 \begin{pmatrix} 1 \\ 0 \end{pmatrix}_j & b(\alpha - \alpha_j) \begin{pmatrix} 1 \\ 0 \end{pmatrix}_j \\ 0 & \frac{\alpha - \alpha_j}{\alpha - \alpha_j + ic} \begin{pmatrix} 1 \\ 0 \end{pmatrix}_j \end{pmatrix}. \tag{3.61}$$

It is now easy to see that $|\omega\rangle$ is an eigenstate of $A(\alpha)$ and $D(\alpha)$

$$A(\alpha)|\omega\rangle = |\omega\rangle \tag{3.62}$$

$$D(\alpha)|\omega\rangle = \prod_{j=1}^{N} \frac{\alpha - \alpha_j}{\alpha - \alpha_j + ic} |\omega\rangle. \tag{3.63}$$

We will now find all the eigenstates of $Z(\alpha)$ by considering the states that are formed by repeated action of the flipping operator B on the ferromagnetic eigenstate (see appendix A for details):

$$\begin{aligned} &(A(\alpha) + D(\alpha)) B(\beta_1) B(\beta_2) |\omega\rangle = \lambda(\alpha, \beta_1, \beta_2) B(\beta_1) B(\beta_2) |\omega\rangle \\ &+ \lambda_1(\alpha, \beta_1, \beta_2) B(\alpha) B(\beta_2) |\omega\rangle + \lambda_2(\alpha, \beta_1, \beta_2) B(\alpha) B(\beta_1) |\omega\rangle \end{aligned} . \tag{3.64}$$

Here

$$\lambda(\alpha, \beta_1, \beta_2) = u(\beta_1 - \alpha) u(\beta_2 - \alpha) + \Delta(\alpha) u(\alpha - \beta_1) u(\alpha - \beta_2) \tag{3.65}$$

$$\lambda_1(\alpha, \beta_1, \beta_2) = v(\beta_1 - \alpha)[u(\beta_2 - \beta_1) - u(\beta_1 - \beta_2)\Delta(\beta_1)] \tag{3.66}$$

$$\lambda_2(\alpha, \beta_1, \beta_2) = v(\beta_2 - \alpha)[u(\beta_1 - \beta_2) - u(\beta_2 - \beta_1)\Delta(\beta_2)]. \tag{3.67}$$

If we want $B(\beta_1)B(\beta_2)|\omega\rangle$ to be an eigenstate of Z we have to choose β_1 and β_2 in such a way that we fulfill the following equations:

$$\lambda_\gamma(\alpha, \beta_1, \beta_2) = 0 \quad \gamma = 1, 2. \tag{3.68}$$

It is straightforward to generalize this to arbitrary M: $B(\beta_1)\cdots B(\beta_M)|\omega\rangle$ is an eigenstate of $Z(\alpha) = A(\alpha) + B(\alpha)$ with eigenvalue

$$\lambda(\alpha, \beta_1, \cdots, \beta_M) = \prod_{\gamma=1}^{M} u(\beta_\gamma - \alpha) + \Delta(\alpha) \prod_{\gamma=1}^{M} u(\alpha - \beta_\gamma) \tag{3.69}$$

if we choose our $\beta_1 \cdots \beta_M$ such that our unwanted terms disappear i.e.

$$\lambda_\gamma(\alpha, \beta_1, \cdots, \beta_M) = 0, \quad \gamma = 1, \cdots, M \ . \tag{3.70}$$

Here

$$\lambda_\gamma(\alpha, \beta_1, \cdots, \beta_M) = v(\beta_\gamma - \alpha) \left(\prod_{\delta=1, \delta\neq\gamma}^{M} u(\beta_\delta - \beta_\gamma) - \Delta(\beta_\gamma) \prod_{\delta=1, \delta\neq\gamma}^{M} u(\beta_\gamma - \beta_\delta) \right) \tag{3.71}$$

$$z_j \equiv \lambda(\alpha_j, \beta_1, \cdots, \beta_M) = \prod_{\gamma=1}^{M} \frac{\beta_\gamma - \alpha_j + iU/2}{\beta_\gamma - \alpha_j} \tag{3.72}$$

and our parameters $\beta_1 \cdots \beta_M$ satisfy the following conditions

$$\prod_{\delta=1, \delta\neq\gamma}^{M} \frac{\beta_\delta - \beta_\gamma + iU/2}{\beta_\delta - \beta_\gamma - iU/2} = \prod_{j=1}^{N} \frac{\beta_\gamma - \alpha_j}{\beta_\gamma - \alpha_j + iU/2}.$$

To make our equations more pleasing to the eye we change variables to $\beta_\gamma = \Lambda_\gamma - iU/4$ recalling that our periodic boundary conditions require that $z_j = e^{-ik_j L}$. Noting that for the Hubbard model $\alpha_j = \sin k_j$, we finally obtain the following equations:

$$e^{ik_j L} = \prod_{\gamma=1}^{M} \frac{\Lambda_\gamma - \sin k_j - iU/4}{\Lambda_\gamma - \sin k_j + iU/4} \tag{3.73}$$

and

$$\prod_{\delta=1, \delta\neq\gamma}^{M} \frac{\Lambda_\delta - \Lambda_\gamma + iU/2}{\Lambda_\delta - \Lambda_\gamma - iU/2} = \prod_{j=1}^{N} \frac{\Lambda_\gamma - \sin k_j - iU/4}{\Lambda_\gamma - \sin k_j + iU/4}. \tag{3.74}$$

These equations are known as the Bethe-Ansatz equations (BAE). Having derived them, we have reached our goal in this section.

3.5 The ground state solution to the BAE

The next step after deriving an equation is of course to try to solve it and obtain the ground state energy. This we will do in this section. The first step is to take the logarithm of

eqns. (3.73) and (3.74). We then obtain the following two transcendental equations:

$$Lk_j = 2\pi n_j + \sum_{\delta=1}^{M} \Theta(2\sin k_j - 2\Lambda_\delta) \tag{3.75}$$

$$\sum_{j=1}^{N} \Theta(2\Lambda_\gamma - 2\sin k_j) = -2\pi I_\gamma + \sum_{\delta=1}^{M} \Theta(\Lambda_\gamma - \Lambda_\delta), \tag{3.76}$$

with

$$\Theta(x) = -2\arctan(2x/u), \quad -\pi \leq \Theta \leq \pi. \tag{3.77}$$

The quantum numbers n_j and I_γ label our states. n_j are integers if M is even and half-odd integers if M is odd. They will take values between the upper and lower bounds $\pm(L-1)/2$. I_γ are integers when $N-M-1$ are even and half-odd integers when $N-M-1$ is odd. They will take values between the upper and lower bounds $\pm(N-M-1)/2$. The energy and momentum of the state is given by

$$P = \sum_{j=1}^{N} k_j = \frac{2\pi}{L}\left(\sum_{j=1}^{N} n_j + \sum_{\gamma=1}^{M} I_\gamma\right) \tag{3.78}$$

$$E = \sum_{j=1}^{N} -2\cos k_j. \tag{3.79}$$

For the ground state n_j and I_γ are consecutive integers or half-integers centered around the origin. We know that k_j takes values in the interval $[-\pi, \pi]$ since k and $k + 2\pi n$ define the same wave function. If we think of n_j as a function of k then $n_j(k+dk) - n_j(k)$ counts the number of k values between k and $k+dk$ so we have that

$$\frac{dn(k)}{dk} = L\rho(k), \tag{3.80}$$

with L the length of that system, and $\rho(k)$ a density. In the same way we have that

$$\frac{dI(\Lambda)}{d\Lambda} = L\sigma(\Lambda). \tag{3.81}$$

We have the obvious normalization for our densities

$$\int_{-Q}^{Q} \rho(k)dk = N/L = n_\uparrow + n_\downarrow = n, \tag{3.82}$$

$$\int_{-B}^{B} \sigma(\Lambda)d\Lambda = M/L = n_\downarrow. \tag{3.83}$$

Here

$$n_\alpha \equiv \frac{1}{L}\sum_{i=1}^{L} \langle \hat{n}_{i\alpha} \rangle \qquad \alpha = \uparrow, \downarrow . \tag{3.84}$$

Note that translational invariance implies that $n_{i\alpha} = n_\alpha$. If we take the derivative of eqn. (3.75) w.r.t. k_j and of eqn. (3.76) w.r.t. Λ_α, setting $dn_j/dk = L\rho(k)$, $dI_\gamma/d\Lambda = L\sigma(\Lambda)$, and then let $N \to \infty$, we obtain the Lieb-Wu equations [22]:

$$\rho(k) = \frac{1}{2\pi} + \cos k \int_{-B}^{B} K^1(\sin k - \Lambda)\sigma(\Lambda)d\Lambda \tag{3.85}$$

$$\sigma(\Lambda) = \int_{-Q}^{Q} K(\sin k - \Lambda)\rho(k)dk - \int_{-B}^{B} K^2(\Lambda - \Lambda')\sigma(\Lambda')d\Lambda'. \tag{3.86}$$

Here

$$K^1(\Lambda - \Lambda') = -\frac{1}{\pi}\theta(2\Lambda - 2\Lambda') = \frac{1}{2\pi}\left(\frac{8U}{U^2 + 16(\Lambda - \Lambda')^2}\right) \tag{3.87}$$

$$K^2(\Lambda - \Lambda') = -\frac{1}{2\pi}\theta(\Lambda - \Lambda') = \frac{1}{2\pi}\left(\frac{4U}{U^2 + 4(\Lambda - \Lambda')^2}\right) = \int_{-\infty}^{\infty} K^1(\Lambda - x)K^1(x - \Lambda')dx. \tag{3.88}$$

The ground state energy now attains the form

$$E = -2L\int_{-Q}^{Q} \rho(k)\cos k dk. \tag{3.89}$$

The Lieb-Wu equations are only solvable on closed form if $Q = \pi$ and $B = \infty$, which corresponds to half-filling n=1. Since $Q > \pi/2$ we observe that $(\cos k)K^1(\sin k - \Lambda)$ is an odd function of $k - \pi/2$ for all Λ and it follows from eqn. (3.85) that $\rho(k) - 1/2\pi$ is also an odd function. On the other hand, $K(\sin k - \Lambda)$ in eqn. (3.86) is an even function of $k - \pi/2$. As a result $\rho(k)$ appearing in the first term of the right-hand side of eqn. (3.86) can be replaced by $1/2\pi$ in the intervall $Q' < k < Q$ and $-Q < k < -Q'$, where $Q' = \pi - Q$. If we now use that $Q = \pi$ and insert eqn. (3.85) into eqn. (3.86) and replace $\rho(k)$ with $1/2\pi$ we obtain the following integral equation for $\sigma_0(\Lambda)$:

$$\sigma_0(\Lambda) = \frac{1}{2\pi}\int_{-\pi}^{\pi} K^1(\sin k - \Lambda)dk - \int_{-\infty}^{\infty} K^2(\Lambda - \Lambda')\sigma_0(\Lambda')d\Lambda'. \tag{3.90}$$

The Fourier transform of eqn. (3.90) is given by

$$\sigma_0(\omega) = \int_{-\infty}^{\infty} e^{i\omega\Lambda}\sigma_0(\Lambda)d\Lambda = \frac{J_0(\omega)}{\cosh(\omega U/4)}. \tag{3.91}$$

We invert this and find

$$\sigma_0(\Lambda) = \frac{1}{2\pi}\int_0^{\infty} \frac{J_0(\omega)\cos(\omega\Lambda)}{\cosh(\omega U/4)}. \tag{3.92}$$

This can be inserted into eqn. (3.85) and we then obtain

$$\rho_0(k) = \frac{1}{2\pi} + \frac{\cos k}{\pi}\int_0^{\infty} \frac{cos(\omega \sin k)J_0(\omega)}{1 + e^{\omega U/2}}. \tag{3.93}$$

If we insert this into eqn. (3.89) we finally obtain for the ground state energy:

$$\frac{E_0}{L} = -4\int_0^{\infty} \frac{J_0(\omega)J_1(\omega)}{\omega(1 + e^{\omega U/2})}d\omega. \tag{3.94}$$

3.6 Magnetic field

In this section we will study the effect that a magnetic field has on the ground state energy. In the presence of a magnetic field the Hubbard model becomes:

$$H = -t\sum_{i=1}^{L}(\hat{c}_{ia}^{\dagger}\hat{c}_{i+1a} + h.c.) + U\sum_{i=1}^{L}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} - \frac{h}{2}\sum_{i=1}^{L}(\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow}). \tag{3.95}$$

The magnetic field wants to force all the spins to be in up direction. When we apply the magnetic field our integral equations (3.85) and (3.86) will be modified, and here we choose to study the half-filled case. This corresponds to $Q = \pi$, this can be seen by inserting eqn. (3.85) into eqn. (3.82). The contribution of the magnetic field to the ground state energy is $-h(n_\uparrow - n_\downarrow)/2$. If we use that we have half-filling we can rewrite this as $-h(1-2n_\downarrow)/2$ and by using eqn. (3.83) we find

$$-\frac{h}{2}(n_\uparrow - n_\downarrow) = -\frac{h}{2} + h\int_{-B}^{B}\sigma(\Lambda)d\Lambda. \tag{3.96}$$

If we now combine eqns. (3.82),(3.89) and (3.96) we obtain the ground state energy

$$\frac{E}{L} = -\frac{h}{2} + \int_{-B}^{B}d\Lambda\sigma(\Lambda)\left[h - 2t\int_{-\pi}^{\pi}\cos^2 kK^1(\Lambda - \sin k)\right] \tag{3.97}$$

$$\sigma(\Lambda) = \frac{1}{2\pi}\int_{-\pi}^{\pi}K^1(\Lambda - \sin k)dk - \int_{-B}^{B}K^2(\Lambda - \Lambda')\sigma(\Lambda')d\Lambda'. \tag{3.98}$$

The integral equation for $\sigma(\Lambda)$ is obtained by inserting eqn. (3.85) into eqn. (3.86). In the next step we rewrite these equations in an operator notation:

$$\langle\Lambda|\hat{\sigma}\rangle = \langle\Lambda|\hat{f}\rangle - \int_{-B}^{B}\langle\Lambda|\hat{K}^2|\Lambda'\rangle\langle\Lambda'|\hat{\sigma}\rangle d\Lambda'. \tag{3.99}$$

Here

$$\sigma(\Lambda) \equiv \langle\Lambda|\hat{\sigma}\rangle \tag{3.100}$$

$$\frac{1}{2\pi}\int_{-\pi}^{\pi}K^1(\Lambda - \sin k)dk \equiv \langle\Lambda|\hat{f}\rangle \tag{3.101}$$

$$K^2(\Lambda - \Lambda') \equiv \langle\Lambda'|\hat{K}^2|\Lambda\rangle \tag{3.102}$$

We now define $\hat{R}$ as the resolvent to $\hat{K}^2$. It has the property that

$$(\hat{1} + \hat{R})(\hat{1} + \hat{K}^2) = \hat{1}. \tag{3.103}$$

Our goal is next to reformulate our problem such that we have an integral equation from B to ∞ instead of $-B$ to B. The way to do this is to use the properties of our resolvent operator. Our functions are defined for all values of Λ so they will not cause any trouble. We start by introducing functions extended to the interval $[-B_0, B_0]$ and denote them with a prime. We also introduce a projection operator $\hat{P}$ which we define as follows:

$$\langle\Lambda|\hat{P}\hat{f}\rangle = \begin{cases} \langle\Lambda|\hat{f}\rangle & -B \le \Lambda \le B \\ 0 & B \le \Lambda \le B_0 \text{ or } -B_0 \le \Lambda \le -B \end{cases} \tag{3.104}$$

We write the extended eqn. (3.98) as

$$\hat{\sigma}' = \hat{f}' - \hat{K}'\hat{P}\hat{f}'. \tag{3.105}$$

If we now add and subtract $\hat{K}'\hat{\sigma}'$ to eqn. (3.105), it can be reformulated as

$$(\hat{1} + \hat{K}')\hat{\sigma}' = \hat{f}' + \hat{K}'(\hat{1} - \hat{P})\hat{\sigma}'. \tag{3.106}$$

Multiplying both sides in eqn. (3.106) by $(\hat{1} + \hat{R}')$,

$$(\hat{1} + \hat{R}')(\hat{1} + \hat{K}')\hat{\sigma} = (\hat{1} + \hat{R}')\hat{f}' + (\hat{1} + \hat{R}')\hat{K}'(\hat{1} - \hat{P})\hat{\sigma}', \tag{3.107}$$

this is equivalent to

$$\hat{\sigma}' = (\hat{1} + \hat{R}')\hat{f}' - \hat{R}'(\hat{1} - \hat{P})\hat{\sigma}'. \tag{3.108}$$

As can be shown by a lengthy calculation [28],

$$(\hat{1} + \hat{R}')\hat{f}' = \hat{\sigma}_0. \tag{3.109}$$

It follows from eqns. (3.108) and (3.109) that

$$\hat{\sigma}' = \hat{\sigma}_0 - \hat{R}(\hat{1} - \hat{P})\hat{\sigma}'. \tag{3.110}$$

If we now let $B_0 \to \infty$ according to eqn. (3.110) we find that eqn. (3.98) transforms as

$$\begin{aligned} \sigma(\Lambda) &= \sigma_0(\Lambda) - \int_{-\infty}^{-B} \frac{4}{U} R\left(\frac{4(\Lambda - \Lambda')}{U}\right) \sigma(\Lambda')d\Lambda' \\ &- \int_{B}^{\infty} \frac{4}{U} R\left(\frac{4(\Lambda - \Lambda')}{U}\right) \sigma(\Lambda')d\Lambda'. \end{aligned} \tag{3.111}$$

Since $\sigma(\Lambda)$ is an even function [33] we can rewrite this as

$$\sigma(\Lambda) = \sigma_0(\Lambda) - \int_{B}^{\infty} \frac{4}{U}\left[R\left(\frac{4(\Lambda - \Lambda')}{U}\right) + R\left(\frac{4(\Lambda + \Lambda')}{U}\right)\right] \sigma(\Lambda')d\Lambda' \tag{3.112}$$

with

$$\sigma_0(\Lambda) \equiv \frac{1}{2\pi}\int_{-\pi}^{\pi} \frac{1}{U}\mathrm{sech}\left(\frac{2\pi(\Lambda - \sin k)}{U}\right) dk. \tag{3.113}$$

This is the solution for $\sigma(\Lambda)$ when $h = 0$, i.e. $B = \infty$. Now we will take a look at the behavior of $\sigma_0(\Lambda)$:

$$\begin{aligned} \sigma_0(\Lambda) &= \frac{1}{2\pi}\int_{-\pi}^{\pi} \frac{2}{U}\exp\left(-\frac{2\pi(\Lambda - \sin k)}{U}\right) dk \\ &= \frac{2}{U}\exp\left(-\frac{2\pi\Lambda}{U}\right)\frac{1}{2\pi}\int_{-\pi}^{\pi} \exp\left(\frac{2\pi\cos k}{U}\right) dk \\ &= \frac{2}{U}I_0(\frac{2\pi}{U})\exp\left(-\frac{2\pi\Lambda}{U}\right). \end{aligned} \tag{3.114}$$

Given this expression for $\sigma_0(\Lambda)$, we can rewrite eqn. (3.112) as

$$\begin{aligned}\sigma(\Lambda) &+ \int_B^\infty \frac{4}{U}\left[R\left(\frac{4(\Lambda-\Lambda')}{U}\right)+R\left(\frac{4(\Lambda+\Lambda')}{U}\right)\right]\sigma(\Lambda')d\Lambda' \\ &= \frac{2}{U}I_0(\frac{2\pi}{U})\exp\left(-\frac{2\pi\Lambda}{U}\right). \end{aligned} \tag{3.115}$$

If we now set $p(x)=\frac{U}{2}\exp(2\pi B/U)\,\sigma(xU/4+B)/I_0(2\pi/U)$ we obtain

$$p(x)=e^{-\frac{\pi x}{2}}-\int_0^\infty\left(R(x-x')+R\left(x+x'+\frac{2B}{U}\right)\right)p(x')dx'. \tag{3.116}$$

If the kernel $R\left(x+x'+\frac{2B}{U}\right)$ is sufficiently small when $x>0$ we can solve the integral equation by introducing a rapidly converging series,

$$p(x)=\sum_{n=1}^\infty p_n(x). \tag{3.117}$$

Here the function $p_n(x)$ fulfills the equation

$$p_n(x) = p_n^{(0)}(x)+\int_0^\infty R(x-x')p_n(x')dx', \tag{3.118}$$

where

$$p_0^{(0)}(x) = e^{-\frac{\pi x}{2}} \tag{3.119}$$

$$p_n^{(0)}(x) = \int_0^\infty R\left(x+x'+\frac{2B}{U}\right)p_{n-1}(x')dx' \quad n\geq 1. \tag{3.120}$$

The $p_n(x)$ equations in (3.135 are of Wiener-Hopf type and can be solved using the Wiener-Hopf method introduced in the appendix. In a similar way we can rewrite the energy as

$$\begin{aligned}\frac{E}{L} &= \frac{E_0}{L}-hI_0\left(\frac{2\pi}{U}\right)\exp\left(\frac{-2\pi B}{U}\right)\int_0^\infty p(x)dx \\ &+ I_0\left(\frac{2\pi}{U}\right)I_1\left(\frac{2\pi}{U}\right)\exp\left(-\frac{4\pi B}{U}\right)\int_0^\infty e^{-\pi x/2}p(x)dx. \end{aligned} \tag{3.121}$$

3.7 Large-U expansion in the repulsive Hubbard model

We shall now investigate what happens if we move away from half filling, i.e. $Q\neq\pi$. In this case we cannot solve the Lieb-Wu equations in closed form so we have to expand them in a Taylor series for large U. We introduce $u\equiv U/4$, with the Lieb-Wu equations taking (3.85) and (3.86) the form

$$2\pi\rho(k) = 1+2u\cos k\int_{-\infty}^\infty\frac{d\Lambda\sigma(\Lambda)}{u^2+(\sin k-\Lambda)^2}, \tag{3.122}$$

and

$$2\pi\sigma(\Lambda) = 2u\int_{-Q}^Q\frac{dk\rho(k)}{u^2+(\sin k-\Lambda)^2}-u\int_\infty^\infty\frac{d\Lambda'\sigma(\Lambda')}{u^2+(\Lambda-\Lambda')^2/4}, \tag{3.123}$$

respectively, with the normalization conditions

$$\int_{-Q}^{Q} dk\rho(k) = N/L = n, \tag{3.124}$$

$$\int_{-\infty}^{\infty} d\Lambda\sigma(\Lambda) = N/L = n_{\downarrow}. \tag{3.125}$$

In exact analogy with the half-filled case we can solve eqn. (3.123) by Fourier transformation and we obtain

$$\sigma(\Lambda) = \frac{1}{4u}\int_{-Q}^{Q} dk\rho(k)\mathrm{sech}\left(\frac{\pi}{2u}(\Lambda - \sin k)\right). \tag{3.126}$$

If we now insert this into eqn. (3.122) we obtain

$$2\pi\rho(k) = 1 + \cos k\int_{-Q}^{Q} dk'\Gamma(k,k')\rho(k'). \tag{3.127}$$

Here

$$\Gamma(k,k') = \frac{1}{2}\int_{-\infty}^{\infty} d\Lambda\frac{\mathrm{sech}\left(\frac{\pi}{2u}(\Lambda + \sin k - \sin k')\right)}{u^2 + \Lambda^2}. \tag{3.128}$$

To simplify the large U expansion we introduce the identity

$$\mathrm{sech}\left(\frac{\pi x}{2u}\right) = \frac{1}{\pi}\int_0^{\infty} dy\cos(xy/2u)\mathrm{sech}(y/2). \tag{3.129}$$

With $x = \Lambda + \sin k - \sin k'$ we obtain

$$\Gamma(k,k') = \frac{1}{u}\int_0^{\infty} dy\frac{\cos\left((\sin k - \sin k')y/2u\right)}{1+e^y}. \tag{3.130}$$

Expanding eqn. (3.130) in $1/u$ one obtains

$$\begin{aligned}\Gamma(k,k') &= \frac{1}{u}\int_0^{\infty}\frac{dy}{1+e^y}\left(1 - \left(\frac{(\sin k - \sin k')y}{2u}\right)^2 + \left(\frac{(\sin k - \sin k')y}{2u}\right)^4 + \cdots\right) \\ &= \frac{1}{u}\int_0^{\infty}\frac{dy}{1+e^y}\left(1 + \sum_{l=1}^{\infty}\frac{(-1)^l y^{2l}}{(2l)!}\left(\frac{\sin k - \sin k'}{2u}\right)^{2l}\right).\end{aligned} \tag{3.131}$$

From ref. [34] we have the following integrals

$$\int_0^{\infty}\frac{dy}{1+e^y} = \ln 2 \tag{3.132}$$

$$\int_0^{\infty}\frac{y^{2l}dy}{1+e^y} = (1 - 2^{-2l})\zeta(2l+1)\Gamma(2l+1). \tag{3.133}$$

Using eqns. (3.132) and (3.133) we can rewrite eqn. (3.131) as

$$\begin{aligned}\Gamma(k,k') &= \frac{1}{u}\left(\ln 2 + \sum_{l=1}^{\infty}(-1)^l(1-2^{-2l})\zeta(2l+1)\left(\frac{\sin k - \sin k'}{2u}\right)^{2l}\frac{\Gamma(2l+1)}{(2l)!}\right) \\ &= \frac{1}{u}\left(\ln 2 + \sum_{l=1}^{\infty}(-1)^l(1-2^{-2l})\zeta(2l+1)\left(\frac{\sin k - \sin k'}{2u}\right)^{2l}\right).\end{aligned} \tag{3.134}$$

Since we are interested in $\rho(k)$ we insert this into eqn. (3.127):

$$\begin{aligned} 2\pi\rho(k) &= 1+\frac{\cos k}{u}\int_{-Q}^{Q}\ln 2\rho(k) \\ &+ \frac{\cos k}{u}\sum_{l=1}^{\infty}(-1)^l(1-2^{-2l})\zeta(2l+1)\int_{-Q}^{Q}dk'\rho(k')\left(\frac{\sin k-\sin k'}{2u}\right)^{2l}. \end{aligned} \tag{3.135}$$

By introducing

$$M_m = \int_{-Q}^{Q}dk'\rho(k')(\sin k')^{2m}, \tag{3.136}$$

we can rewrite $\rho(k)$ in eqn. (3.135) as

$$\begin{aligned} 2\pi\rho(k) &= 1+\frac{\cos k}{u}n\ln 2 \\ &+ \frac{\cos k}{u}\sum_{l=1}^{\infty}(-1)^l(1-2^{-2l})\zeta(2l+1)\sum_{m=0}^{l}\left(\begin{array}{c}2l\\2m\end{array}\right)M_m(\sin k)^{2(l-m)}. \end{aligned} \tag{3.137}$$

To get a formula for M_m we multiply by $(\sin k)^{2m}$ and integrate over k:

$$\begin{aligned} \int_{-Q}^{Q}\rho(k)(\sin k)^{2m}dk &= \frac{1}{2\pi}\int_{-Q}^{Q}(\sin k)^{2m}dk+\frac{n\ln 2}{2\pi u}\int_{-Q}^{Q}\cos k(\sin k)^{2l}dk \\ &+ \frac{1}{2\pi u}\sum_{l=1}^{\infty}(-1)^l(1-2^{-2l})\zeta(2l+1) \\ &\times \sum_{\nu=0}^{l}\left(\begin{array}{c}2l\\2\nu\end{array}\right)\int_{-Q}^{Q}M_\nu\cos k(\sin k)^{2(l+m-\nu)}dk. \end{aligned} \tag{3.138}$$

If we now use the identity

$$\int_{-Q}^{Q}\cos k(\sin k)^{2m}dk = \frac{(\sin Q)^{2m+1}}{2m+1}, \tag{3.139}$$

we obtain the following equation for M_m

$$\begin{aligned} M_m &= \frac{1}{2\pi}\int_{-Q}^{Q}(\sin k)^{2m}dk+\frac{n\ln 2}{\pi u}(\sin Q)^{2l+1}/(2n+1) \\ &+ \frac{1}{\pi u}\sum_{l=1}^{\infty}(-1)^l(1-2^{-2l})\zeta(2l+1) \\ &\times \sum_{\nu=0}^{l}\left(\begin{array}{c}2l\\2\nu\end{array}\right)M_\nu(\sin Q)^{2(l+m-\nu)+1}/(2(l+m-\nu)+1). \end{aligned} \tag{3.140}$$

One can now solve this equations iteratively and this is done in [27] and from this result one obtains an expansion for the ground state energy. We will only present the result here:

$$\frac{E}{L} = -\frac{2}{\pi}\sin(\pi n)-\sum_{l=1}^{\infty}\kappa_l(n)(1/U)^l. \tag{3.141}$$

The first few terms in $\kappa_l(n)$ are given in tab. (3.1)

Table 3.1: First five coefficients of $\kappa_l(n)$. Notation $A = 4\ln 2$, $s = \sin(\pi n)$ and $f = \sin(2\pi n)/(2\pi n)$

l	$\kappa_l(n)$
1	$An^2(1-f)$
2	$-\pi^{-1}A^2n^2s^3$
3	$(4/3)A^3n^4s^2f + \zeta(3)n^2[3(1-f)(2f-3) + 2s^2f]$
4	$\pi^{-1}An^2s^3\{4\zeta(3)[5(1-f)+2s^2] - (5/12)A^3n^2(4-5s^2\}$
5	$(2/5)A^5n^6s^2f(5-9s^2) - 4\zeta(3)A^2n^4s^2\{3f[3(1-f)+2s^2] + 4s^4/(\pi n)^2\}$
	$+\zeta(5)n^2\{15(1-f)[5-(3/2)(3+2s^2)f] - (5+4s^2)s^2f\}$

Chapter 4

Entanglement in the Hubbard model

In this chapter we will study entanglement in the Hubbard model. We will start with the simplest case when we only have a hopping term and an on-site interaction:

$$H = -t\sum_{i=1}^{L}(\hat{c}_{ia}^{\dagger}\hat{c}_{i+1a} + h.c.) + U\sum_{i=1}^{L}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}. \tag{4.1}$$

This Hamiltonian was diagonalized on closed form in the previous chapter and we will now perform an analysis of the entanglement in the ground state for $-\infty \leq U \leq \infty$. These results were first calculated in [9] and we will reproduce the calculation here. Later in this chapter we will add a chemical potential and a magnetic field to our Hamiltonian, and calculate the resulting entanglement.

4.1 A starting point

As a starting point we fix the filling to $n = 1$ (half-filled band). The ground state will be a spin singlet [35] which means that we will have the same number of spin up as spin down i.e. $\langle\hat{n}_{i\uparrow}\rangle = \langle\hat{n}_{i\downarrow}\rangle = 1/2$. As we mentioned earlier, the parameters in our calculation of the local entanglement in the Hubbard model are given by

$$\omega = \frac{1}{L}\frac{\partial E}{\partial U} \tag{4.2}$$

$$u^{+} = \langle\hat{n}_{i\uparrow}\rangle - \omega = \frac{1}{2} - \omega \tag{4.3}$$

$$u^{-} = \langle\hat{n}_{i\downarrow}\rangle - \omega = \frac{1}{2} - \omega \tag{4.4}$$

$$z = 1 - u^{+} - u^{-} - \omega = \omega. \tag{4.5}$$

This implies that we can write the von Neumann entropy as

$$E_{\nu}(\omega) = -2\omega\log_2\omega - 2(1/2-\omega)\log_2(1/2-\omega). \tag{4.6}$$

It is now time to calculate the double occupancy ω. We start with the ground state energy which we calculated in the previous chapter (cf. eqn. (3.94)):

$$\frac{E_0}{L} = -4t\int_0^{\infty} dp \frac{J_0(p)J_1(p)}{p(1+e^{\frac{U}{2t}|p|})}. \tag{4.7}$$

Combining eqns. (4.2) and (4.7) it follows that

$$\begin{aligned}\omega &= \frac{\partial}{\partial U}\left(-4t\int_0^\infty dp\frac{J_0(p)J_1(p)}{p(1+e^{\frac{U}{2t}|p|})}\right) = 2\int_0^\infty dp\frac{J_0(p)J_1(p)p|p|e^{\frac{U}{2t}|p|}}{p^2(1+e^{\frac{U}{2t}|p|})^2} \\ &= \int_0^\infty dp\frac{J_0(p)J_1(p)}{1+\cosh(\frac{U}{2t}|p|)}. \end{aligned} \tag{4.8}$$

We can obtain the case $U<0$ by calculating the case $U>0$ and then use the particle-hole transformation [24]

$$\hat{c}^\dagger_{i\uparrow} = (-1)^i\hat{a}_{i\uparrow} \qquad \hat{c}^\dagger_{i\downarrow} = (-1)^i\hat{a}_{i\downarrow} \tag{4.9}$$

$$\hat{c}_{i\uparrow} = (-1)^i\hat{a}^\dagger_{i\uparrow} \qquad \hat{c}_{i\downarrow} = (-1)^i\hat{a}^\dagger_{i\downarrow}. \tag{4.10}$$

This transformation will be investigated in detail in chapter 5 and there it will be shown that we obtain the following relation for the ground state energy between the repulsive and the attractive cases:

$$\begin{aligned}E_0(N-M,M;U) &= (N-M)U + E_0(N-M,L-M;-U) \\ &= -(L-N)U + E_0(L-N+M,L-M;U). \end{aligned} \tag{4.11}$$

Now we note that for half-filling, i.e. N=L and M=N/2, we have that

$$E_0(N/2,N/2;U) = (N/2)U + E_0(N/2,N/2;-U). \tag{4.12}$$

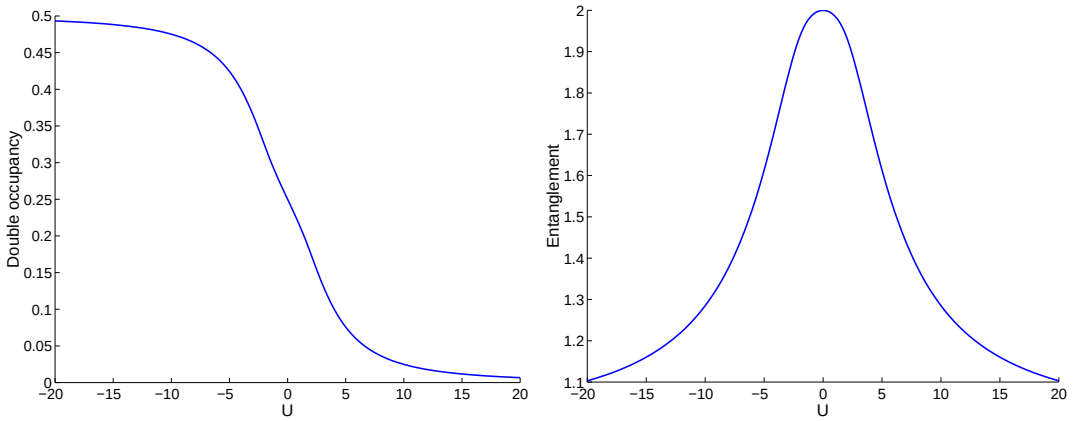
Since we are interested in ω we differentiate eqn. (4.12):

$$\frac{1}{L}\frac{\partial}{\partial U}\left(E_0(N/2,N/2;U)\right) = \frac{1}{L}\frac{\partial}{\partial U}\left((N/2)U + E_0(N/2,N/2;-U)\right). \tag{4.13}$$

It follows from eqns. (4.2) and (4.13) that

$$\omega(-U) = \frac{1}{2} - \omega(U). \tag{4.14}$$

Note that this implies that entanglement is an even function: $E_\nu(U) = E_\nu(-U)$. (This can be easily seen by inserting our result from eqn. (4.14) into eqn. (4.6).) The result for $\omega(U)$, plotted in fig. (4.1(a)), is what we expect when U is large: Almost all of our sites are singly occupied. When -U is large we have that almost half of our sites are doubly occupied and the rest are empty. If we take a look at the behavior of the local entanglement, as plotted in fig. (4.1(b)), we see that it has a maximum at the point $U=0$, which is the Mott transition point. Our numerical plot of E_ν and ω are obtained for U in the interval $-20 \leq U \leq 20$. What happens if we extend our study beyond this interval? We start with the limit $U\to\infty$. Here there is no double occupancy, so $E_\nu(\omega)=1$ since $\omega=0$ and $u^+ = u^- = 1/2$. When U decreases and becomes finite the hopping between sites leads to an appearance of doubly occupied sites. This will increase ω which in turn enhances the entanglement. For $U\to-\infty$ we have that half of the sites are doubly occupied and the other half empty. This will give $\omega = 1/2$ and $E_\nu(\omega)=1$. When U becomes finite in the attractive case the hopping between sites begins and ω starts to decrease. This implies that $E_\nu(\omega)$ will increase. Summing it all up: When $|U|$ increases $E_\nu(\omega)$ decreases and it follows that we have a global maximum of the entanglement at $U=0$, which is the quantum phase transition point (metal-insulator transition).



(a) Double occupancy versus U.

(b) Entanglement versus U.

Figure 4.1:

4.2 Attractive case with magnetic field

We now turn our attention to the case of $U < 0$. In this case the particles want to form local bound pairs (singlets in spin space). This implies that when we apply a magnetic field h we don't get an effect unless $h \geq h_{c1} > 0$ (which defines h_{c1} as a lower critical field). This is a consequence of the fact that one needs a sufficiently large magnetic field (of order $|U| \sim h_{c1}$) so as to split up a bound pair. The Hamiltonian now has the form

$$H = -t\sum_{i=1}^{L}(\hat{c}_{ia}^{\dagger}\hat{c}_{i+1a} + h.c.) + U\sum_{i=1}^{L}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} - \frac{h}{2}\sum_{i=1}^{L}(\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow}). \tag{4.15}$$

We are interested in how the entanglement behaves at the two critical points h_{c1}, when the first spin flips around, and h_{c2} (the upper critical field) when we have full magnetization. We still have that the entanglement can be written on the form

$$E_{\nu}(\rho) = -z\log_2 z - u^{+}\log_2 u^{+} - u^{-}\log_2 u^{-} - \omega\log_2\omega \tag{4.16}$$

since the Hamiltonian in eqn. (4.15) is translational invariant and conserves particle number (fixed at half-filling) as well as the z-component of the total spin. We remind the reader that these three conditions are the ones we imposed in chapter 2 to guarantee the diagonal form of the reduced density matrix. However, the parameters in eqn. (4.16) will now depend on the magnetic field h, so we start by calculating u^{+} and u^{-}. When the magnetization is zero we still have the same parameters as in the case with zero magnetic field, i.e. $u^{+} = u^{-} = 1/2 - \omega$. The change in the number of doubly occupied states are seen from the change in the derivative of the ground state energy with respect to U. However this cannot be calculated for arbitrary values of U since we cannot solve the Lieb-Wu equations on closed form. The problem will be the same as with the repulsive case with a magnetic field analyzed in the previous chapter. In the following, we therefore focus on the tractable limits $U \to -\infty$ and $U \to 0$. As a preliminary, we note that the difference in the number of up and down spins are measured by the magnetization $m = \sum_{i=1}^{L}(n_{i\uparrow} - n_{i\downarrow})/2L$. It follows from eqns. (4.3) and (4.4) that u^{+}

and u^- are given by

$$u^+ = \frac{1}{2} + m - \omega \tag{4.17}$$

$$u^- = \frac{1}{2} - m - \omega. \tag{4.18}$$

Since we are in the half-filled case the number of empty sites are of course the same as the number of doubly occupied sites.

4.3 The large-$|U|$ limit

We start by investigating the large-$|U|$ limit where we have only doubly occupied states when $h = 0$. The corner stone in our entanglement calculation is the ground state energy. This is calculated in ref. [36] and we will only present the result here. The calculation of the ground state energy in [36] is only valid in the region $U \gg 4$ (in the next chapter we will see how we can extend this study to the case $U \geq 4$). In this region one finds [36]:

$$\frac{E}{L} = U\left(\frac{n}{2} - m\right) - \frac{2}{\pi}\sin(2\pi m). \tag{4.19}$$

With this result in our hands we can calculate everything that we need. Let us start with the double occupancy:

$$\omega = \frac{1}{L}\frac{\partial E}{\partial U} = \frac{n}{2} - m. \tag{4.20}$$

Eqns. (4.5), (4.17), (4.18) and (4.20) imply that our parameters at half-filling ($n = 1$) are given by

$$\omega = \frac{1}{2} - m \tag{4.21}$$

$$u^+ = \frac{1}{2} + m - \frac{1}{2} + m = 2m \tag{4.22}$$

$$u^- = \frac{1}{2} - m - \frac{1}{2} + m = 0 \tag{4.23}$$

$$z = 1 - \omega - u^+ - u^- = \frac{1}{2} - m. \tag{4.24}$$

Combining eqns. (4.21)-(4.24) it follows that the von Neumann entropy is given by

$$E_\nu(m) = -2m\log_2(2m) - 2\left(\frac{1}{2} - m\right)\log_2\left(\frac{1}{2} - m\right). \tag{4.25}$$

Rather than having the von Neumann entropy as a function of the magnetization m we would like to have it as a function of the magnetic field. In the region (h_{c1}, h_{c2}) $h(m)$ is invertible and we can use the Hellman-Feynman theorem to calculate the magnetic-field:

$$h = \frac{\partial E}{\partial m} = -U - 4\cos(2\pi m). \tag{4.26}$$

From this we find the magnetization as a function of the magnetic field:

$$m(h) = \begin{cases} 0 & 0 \leq h < h_{c1} \\ \frac{1}{2\pi}\arccos\left(-\frac{U+h}{4}\right) & h_{c1} \leq h \leq h_{c2} \\ \frac{1}{2} & h_{c2} < h \end{cases}. \tag{4.27}$$

How do we find the critical field h_{c1}? From ref. [37] we have that the energy gap between the ground state and the first spin-flipped excited state in the $U \to -\infty$ limit is

$$\Delta E = |U| - 4 \tag{4.28}$$

when $h = 0$. It is easy to realize that the presence of $|U|$ in eqn. (4.28) comes from the prize that we have to pay to split up a pair (which is the same amount that we gain when they are paired up, i.e. U). The -4 in the gap is a bit more surprising but it comes from the fact that in the case $U = -\infty$ we have only particles that are paired up, with half of the sites empty. Clearly, there is no hopping between sites in the ground state since the price for each jump is infinite. In the first excited state we have two particles in the spin up direction and we can now have four jumps in each local state which yield the energy -4 (recall that we have set the hopping amplitude t to unity). It follows that the total energy gap sums up to be $\Delta E = |U| - 4$. We can now calculate the effect that the magnetic field has on this gap. When $U = -\infty$ we only have doubly occupied local states in the ground state. The magnetic energy of these states is clearly zero:

$$-\frac{h}{2}(\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})|\uparrow\downarrow\rangle_i = -\frac{h}{2}(1-1)|\uparrow\downarrow\rangle_i = 0. \tag{4.29}$$

In the first excited state we have two spins in the up direction and these states will be affected by the magnetic field according to

$$-\frac{h}{2}(\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})|\uparrow\rangle_i = -\frac{h}{2}|\uparrow\rangle_i. \tag{4.30}$$

In the first excited state we thus have a total decrease of energy of h which implies that if we turn up the magnetic field to $h = |U| - 4$ we will have a level crossing with a resulting change in the ground state at $h_{c1} = |U| - 4$. We are now ready to calculate the entanglement in the large-U limit as a function of the magnetic field. Putting together eqns. (4.25) and (4.27) we find that

$$\begin{aligned} E_\nu(h) &= -\left(\frac{1}{\pi}\arccos\left(-\frac{U+h}{4}\right)\right)\log_2\left(\frac{1}{\pi}\arccos\left(-\frac{U+h}{4}\right)\right) \\ &- \left(1-\frac{1}{\pi}\arccos\left(-\frac{U+h}{4}\right)\right)\log_2\left(\frac{1}{2}-\frac{1}{2\pi}\arccos\left(-\frac{U+h}{4}\right)\right), \end{aligned} \tag{4.31}$$

with h in the region $h_{c1} \leq h \leq h_{c2}$. To get a clearer understanding of the behavior in this region we plot the entanglement against the magnetic field, see fig. (4.2). Looking at the plot at the two critical points $h_{c1} = -U - 4$ and $h_{c2} = -U + 4$ it seems as if the derivative of the entanglement is divergent. Since we have an analytical expression of the entanglement as a function of h we can investigate if it is divergent or just very large at the two critical points:

$$\begin{aligned} \frac{\partial E_\nu(h)}{\partial h} &= \frac{1}{4\pi\sqrt{1-\left(\frac{U+h}{4}\right)^2}}\left\{-\log_2\left(\frac{1}{\pi}\arccos\left(-\frac{U+h}{4}\right)\right)\right. \\ &+ \left.\log_2\left(\frac{1}{2}-\frac{1}{2\pi}\arccos\left(-\frac{U+h}{4}\right)\right)\right\}. \end{aligned} \tag{4.32}$$

The expression in eqn. (4.32) diverges at the two critical points since when $h \to h_{c1}$ we have that $-(U+h)/4 \to 1$. In the limit $h \to h_{c2}$ we have $-(U+h)/4 \to -1$ and since

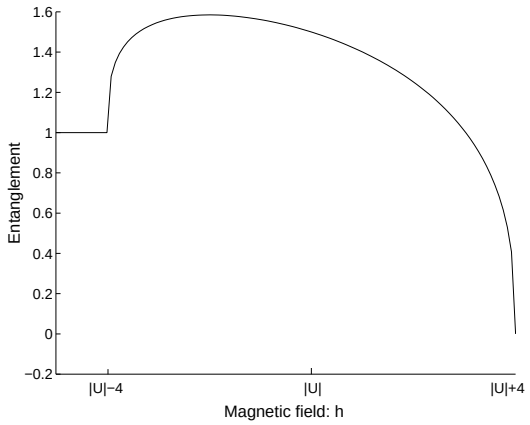


Figure 4.2: Entanglement versus magnetic field at $|U| \to -\infty$.

$\arccos(-1) = \pi$ we have the same divergence as in h_{c1} but with a change in sign. The next question that arises is whether we can express the derivative of the entanglement as a function depending on $h - h_c$? Noting that

$$-\frac{U+h}{4} = 1 - \frac{h-h_{c1}}{4} \tag{4.33}$$

we can rewrite eqn. (4.32) in the limit $h \to h_{c1}$ as

$$\begin{aligned}\frac{\partial E_\nu(h)}{\partial h} &= \frac{1}{4\pi\sqrt{1-\left(\frac{U+h}{4}\right)^2}}\left\{-\log_2\left(\frac{1}{\pi}\arccos\left(1-\frac{h-h_{c1}}{4}\right)\right)\right. \\ &+ \left.\log_2\left(\frac{1}{2}-\frac{1}{2\pi}\arccos\left(1-\frac{h-h_{c1}}{4}\right)\right)\right\}. \end{aligned} \tag{4.34}$$

When $h \to h_{c1}$ we have that $\arccos(1-(h-h_{c1})/4) \to 0$ so the dominating term in our derivative will be the first logarithmic term. The next step is to study the behavior of $\arccos(1-\varepsilon)$:

$$\frac{1}{\pi}\arccos(1-\varepsilon) \simeq \frac{1}{\sqrt{2}\pi}\sqrt{h-h_{c1}} + O\left((h-h_{c1})^{\frac{3}{2}}\right). \tag{4.35}$$

Finally we rewrite the denominator in eqn. (4.34) as

$$1-\left(\frac{U+h}{4}\right)^2 = \frac{h-h_{c1}}{2} - \left(\frac{h-h_{c1}}{4}\right)^2. \tag{4.36}$$

In the limit $h \to h_{c1}$ we can neglect the quadratic term in the right-hand side of eqn. (4.36), and we obtain

$$\frac{1}{\sqrt{1-\left(\frac{U+h}{4}\right)^2}} \sim \frac{\sqrt{2}}{\sqrt{h-h_{c1}}}. \tag{4.37}$$

To summarize in the limit $h \to h_{c1}$ we write the dominating term in eqn. (4.34) as

$$\begin{aligned}\frac{\partial E_\nu(h)}{\partial h} &\simeq -\frac{\sqrt{2}}{4\pi}\frac{1}{\sqrt{h-h_{c1}}}\log_2\left(\frac{1}{\sqrt{2}\pi}\sqrt{h-h_{c1}}\right)\\ &\simeq -\frac{1}{\ln(2)4\sqrt{2}\pi}\frac{1}{\sqrt{h-h_{c1}}}\left(\ln\left(\frac{1}{2\pi^2}(h-h_{c1})\right)+\text{const.}\right)\\ &\simeq -\frac{C}{\sqrt{h-h_{c1}}}\left(\ln\left(h-h_{c1}\right)+\text{const.}\right).\end{aligned} \tag{4.38}$$

In the limit $h \to h_{c2}$ we can use the following identities:

$$\frac{1}{\sqrt{1-\left(\frac{U+h}{4}\right)^2}} \sim \frac{\sqrt{2}}{\sqrt{h_{c2}-h}} \tag{4.39}$$

$$-\frac{U+h}{4} = \frac{h_{c2}-h}{4}-1 \tag{4.40}$$

$$\frac{1}{2\pi}\arccos(\varepsilon-1) \simeq \frac{1}{2}-\frac{\sqrt{2}}{2\pi}\sqrt{\varepsilon}+O\left(\varepsilon^{\frac{3}{2}}\right). \tag{4.41}$$

If we use eqns. (4.39)-4.41 to rewrite eqn. (4.32) we obtain in the limit $h \to h_{c2}$

$$\begin{aligned}\frac{\partial E_\nu(h)}{\partial h} &\simeq \frac{\sqrt{2}}{4\pi\sqrt{h_{c2}-h}}\log_2\left(\frac{1}{2\sqrt{2}\pi}(h_{c2}-h)^{1/2}\right)\\ &= \frac{1}{4\sqrt{2}\ln(2)\pi\sqrt{h_{c2}-h}}\ln\left(\frac{1}{8\pi^2}(h_{c2}-h)\right)\\ &= \frac{C}{\sqrt{h_{c2}-h}}\left(\ln(h_{c2}-h)+\text{const.}\right),\end{aligned} \tag{4.42}$$

here

$$C = \frac{1}{4\sqrt{2}\ln(2)\pi}. \tag{4.43}$$

To identify the origin of the divergent terms we can rewrite the derivative in the "mixed" form:

$$\frac{\partial E_\nu(h)}{\partial h} = -\frac{\partial m}{\partial h}\frac{1}{\ln 2}\left(2\ln(u^+)-\ln(\omega)-\ln(z)\right). \tag{4.44}$$

The logarithmic divergence is caused by the change in the dimension of the local Hilbert space at the transition: when $h \to h_{ci}$ we close one or several local states for the particles. This is what happens in the attractive Hubbard with magnetic field for $U = -\infty$ at h_{c1} where we close the state $|\uparrow\rangle$. Below h_{c1} we only have a mixture of $|\uparrow\downarrow\rangle$ and $|0\rangle$. The first term that can be shown to cause the $1/(\sqrt{|h_c-h|})$ divergence is simply the magnetic susceptibility,

$$\chi = \frac{\partial m}{\partial h}. \tag{4.45}$$

From [36] we have that the susceptibility in the two limits $h \to h_{c1}$ and $h \to h_{c2}$ are given by

$$\chi_{c1} = \frac{1}{2\left(a_2(h-h_{c1})\right)^{1/2}} \tag{4.46}$$

and

$$\chi_{c2} = \frac{1}{2\left(b_2(h_{c2}-h)\right)^{1/2}}, \tag{4.47}$$

respectively. Here

$$a_2 = \left.\frac{\partial^3 E}{\partial m^3}\right|_{m=0}, \qquad b_2 = -\left.\frac{\partial^3 E}{\partial m^3}\right|_{m=1/2}. \tag{4.48}$$

If we use eqn. (4.19) we can easily calculate a_2 and b_2:

$$a_2 = 8\pi^2 \quad , \quad b_2 = 8\pi^2. \tag{4.49}$$

This implies that the susceptibility's are given by

$$\chi_{c1} = \frac{1}{4\sqrt{2}\pi(h-h_{c1})^{1/2}} \quad , \quad \chi_{c2} = \frac{1}{4\sqrt{2}\pi(h_{c2}-h)^{1/2}}. \tag{4.50}$$

It follows from eqns. (4.42) and (4.50) that we can rewrite the derivative of the entanglement on the form

$$\frac{\partial E_\nu(h)}{\partial h} = C_0 \chi \ln(|h_c - h|) \tag{4.51}$$

with $C_0 = 1/\ln 2$.

4.4 Small U-limit

In the limit $|U| \ll 1$ we once again use results from [36] where the ground state energy has been calculated. At half-filling we have that

$$\frac{E}{L} = -\frac{4}{\pi}\cos(m\pi) \tag{4.52}$$

$$\omega = \frac{1}{4} - m^2. \tag{4.53}$$

By the Hellmann-Feynman theorem we get the magnetic field as a function of the magnetization in the critical region.

$$h = \frac{1}{L}\frac{\partial E}{\partial m} = 4\sin(m\pi). \tag{4.54}$$

This implies that the magnetization in the region $h_{c1} \leq h \leq h_{c2}$ is given by:

$$m(h) = \frac{1}{\pi}\arcsin\left(\frac{h}{4}\right) = \frac{1}{2} - \frac{1}{\pi}\arccos\left(\frac{h}{4}\right). \tag{4.55}$$

The reason that we rewrite the magnetization as a function of $\arccos\left(\frac{h}{4}\right)$ is that it will be easier to compare the results here with the large-U limit. The parameters as a function of

the magnetic field h attains the form

$$\omega = \frac{1}{4} - (m(h))^2 = \frac{1}{\pi}\arccos\left(\frac{h}{4}\right) - \frac{1}{\pi^2}\arccos^2\left(\frac{h}{4}\right) \tag{4.56}$$

$$u^+ = \frac{1}{2} + m(h) - \omega = 1 - \frac{2}{\pi}\arccos\left(\frac{h}{4}\right) + \frac{1}{\pi^2}\arccos^2\left(\frac{h}{4}\right) \tag{4.57}$$

$$u^- = \frac{1}{2} - m(h) - \omega = \frac{1}{\pi^2}\arccos^2\left(\frac{h}{4}\right) \tag{4.58}$$

$$z = \omega(h) = \frac{1}{\pi}\arccos\left(\frac{h}{4}\right) - \frac{1}{\pi^2}\arccos^2\left(\frac{h}{4}\right). \tag{4.59}$$

We can now write the von Neumann entropy as a function of h:

$$E_\nu(h) = -2\omega(h)\log_2(\omega(h)) - u^+(h)\log_2(u^+(h)) - u^-(h)\log_2(u^-(h)) \tag{4.60}$$

and by inserting eqns. (4.56)-(4.59) into eqn. (4.60) we can plot $E_\nu(h)$ and this is done in fig. (4.3). If we take a look at the plot in fig. (4.3) of the von Neumann entropy for the $U = 0^-$ case we once again see that we have a very large slope at $h = h_{c2} = 4$. Let ous calculate it analytically:

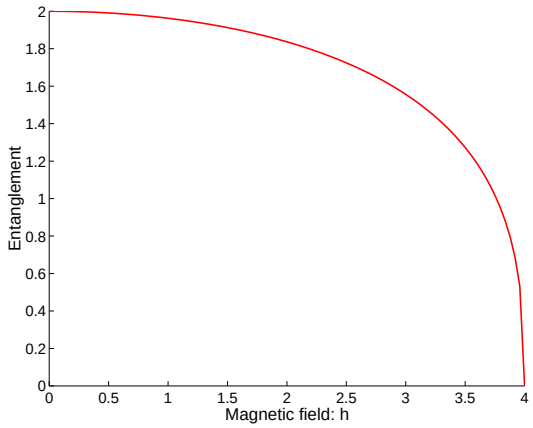


Figure 4.3: Entanglement versus magnetic field at $U = 0$.

$$\begin{aligned}\frac{\partial E_\nu(h)}{\partial h} = \frac{1}{2\pi}\frac{1}{\sqrt{1-\left(\frac{h}{4}\right)^2}}\Bigg\{&\left(\frac{1}{\pi}\arccos\left(\frac{h}{4}\right)\right)\log_2\left(\frac{1}{\pi^2}\arccos^2\left(\frac{h}{4}\right)\right)\\ &+\left(1-\frac{2}{\pi}\arccos\left(\frac{h}{4}\right)\right)\log_2\left(\frac{1}{\pi}\arccos\left(\frac{h}{4}\right)-\frac{1}{\pi^2}\arccos^2\left(\frac{h}{4}\right)\right)\\ &-\left(1-\frac{1}{\pi}\arccos\left(\frac{h}{4}\right)\right)\log_2\left(1-\frac{2}{\pi}\arccos\left(\frac{h}{4}\right)+\frac{1}{\pi^2}\arccos^2\left(\frac{h}{4}\right)\right)\Bigg\}.\end{aligned} \tag{4.61}$$

The following identities will be useful in our further investigation of the derivative at $h_{c2} = 4$:

$$\frac{h}{4} = 1 - \frac{h_{c2} - h}{4} \tag{4.62}$$

$$\varepsilon = \frac{h_{c2} - h}{4} \tag{4.63}$$

$$\frac{1}{\pi}\arccos(1-\varepsilon) = \frac{\sqrt{2}}{\pi}\sqrt{\varepsilon} + O\left(\varepsilon^{\frac{3}{2}}\right). \tag{4.64}$$

We also observe that

$$\begin{aligned}&\left(\frac{1}{\pi}\arccos\left(\frac{h}{4}\right)\right)\log_2\left(\frac{1}{\pi^2}\arccos^2\left(\frac{h}{4}\right)\right)\\&=\left(\frac{2}{\pi}\arccos\left(\frac{h}{4}\right)\right)\log_2\left(\frac{1}{\pi}\arccos\left(\frac{h}{4}\right)\right)\quad\rightarrow\quad 0\end{aligned}\tag{4.65}$$

when $h \rightarrow h_{c2}$. In this limit the dominating terms of eqn. (4.61) will behave as

$$\begin{aligned}\frac{\partial E_\nu(h)}{\partial h} &\simeq \frac{1}{\sqrt{2}\pi\sqrt{h_{c2}-h}}\left(\log_2\left(\frac{1}{\sqrt{2}\pi}\sqrt{h_{c2}-h}\right)+\text{const.}\right)\\&= \frac{1}{2\sqrt{2}\pi\ln(2)\sqrt{h_{c2}-h}}\left(\ln\left(h_{c2}-h\right)+\text{const.}\right)\\&= \frac{C}{\sqrt{h_{c2}-h}}\left(\ln(h_{c2}-h)+\text{const.}\right)\end{aligned}\tag{4.66}$$

here

$$C=\frac{1}{2\sqrt{2}\ln(2)\pi}.\tag{4.67}$$

In the same way as in the Large-U limit we can rewrite this as

$$\frac{\partial E_\nu(h)}{\partial h} = C_0\chi\ln(h_{c2}-h),\tag{4.68}$$

where again we have that $C_0 = 1/\ln 2$.

4.5 Repulsive case with magnetic field

We start by writing down the Hamiltonian for the $U > 0$ Hubbard model in the presence of a magnetic field:

$$H = -t\sum_{i=1}^{L}(\hat{c}_{ia}^\dagger\hat{c}_{i+1a}+h.c.)+U\sum_{i=1}^{L}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}-\frac{h}{2}\sum_{i=1}^{L}(\hat{n}_{i\uparrow}-\hat{n}_{i\downarrow}).\tag{4.69}$$

In the previous chapter we showed that we can't solve the Lieb-Wu equations on closed form. Let us instead focus on what we *can* do: a series expansion in the $h \rightarrow 0$ (i.e. $m = 0$) or $h \rightarrow -h_{c2}$ (i.e. $m \rightarrow -1/2$) limit. We focus our attention on the case $h \rightarrow -h_{c2}$ where we expect that we have a divergence in the derivative. In this limit $B \ll min(1, U)$, and one can expand the ground state energy as a function of $n_{i\uparrow}$. This is done in [38] and we will only present the result here:

$$\begin{aligned}\frac{E}{L} &= -4\left(\sqrt{1+\left(\frac{U}{4}\right)^2}-\frac{U}{4}\right)n_{i\uparrow}\\&+ \frac{\pi^2}{6}\frac{1}{\sqrt{1+(U/4)^2}}n_{i\uparrow}^3+O(n_{i\uparrow}^4).\end{aligned}\tag{4.70}$$

We also have an analytic expression for the case $U = 0^+$

$$\frac{E}{L} = -\frac{4}{\pi} cos(\pi m). \tag{4.71}$$

This is analogous to the $U = 0^-$ case which we analyzed in the previous section. To make the comparison to previous results more transparent, which all have been calculated in the region $h \geq 0$ we use the following relation from [22]:

$$E(N_\uparrow, N_\downarrow, U) = -(L - N)U + E(L - N_\uparrow, L - N_\downarrow, U). \tag{4.72}$$

As expected we see that the ground state energy is an even function w.r.t. magnetization at half-filling. We can now rewrite eqn. (4.70) as

$$\begin{aligned} \frac{E}{L} &= -4\left(\sqrt{1+\left(\frac{U}{4}\right)^2} - \frac{U}{4}\right) n_{i\downarrow} \\ &+ \frac{\pi^2}{6}\frac{1}{\sqrt{1+(U/4)^2}} n_{i\downarrow}^3 + O(n_{i\downarrow}^4). \end{aligned} \tag{4.73}$$

This is the energy in the limit $n_{i\downarrow} \to 0$ (i.e. $m \to 1/2$ and $h \to h_{c2}$). We rewrite the energy in eqn. (4.73) by using the fact that $n_{i\downarrow} = 1/2 - m$:

$$\begin{aligned} \frac{E}{L} &= -4\left(\sqrt{1+(U/4)^2} - \frac{U}{4}\right)\left(\frac{1}{2} - m\right) \\ &+ \frac{\pi^2}{6}\frac{1}{\sqrt{1+(U/4)^2}}\left(\frac{1}{2} - m\right)^3 + O\left(\left(\frac{1}{2} - m\right)^4\right). \end{aligned} \tag{4.74}$$

We can now use the Hellman-Feynman theorem to obtain the magnetic field as a function of magnetization:

$$\begin{aligned} h = \frac{1}{L}\frac{\partial E}{\partial m} &= 4\left(\sqrt{1+(U/4)^2} - \frac{U}{4}\right) \\ &- \frac{\pi^2}{2}\frac{1}{\sqrt{1+(U/4)^2}}\left(\frac{1}{2} - m\right)^2 + O\left(\left(\frac{1}{2} - m\right)^3\right). \end{aligned} \tag{4.75}$$

We can express $n_{i\downarrow}$ as a function of the magnetic field,

$$n_{i\downarrow} = \left(\frac{1}{2} - m\right) = \frac{\sqrt{2\sqrt{1+(U/4)^2}}}{\pi}\sqrt{h_{c2} - h} = C_0\sqrt{h_{c2} - h}. \tag{4.76}$$

We have here used the following relation from [24]:

$$h_{c2} = \sqrt{1+\left(\frac{U}{4}\right)^2} - \frac{U}{4}. \tag{4.77}$$

Rewriting eqn. (4.76) we obtain for the magnetic susceptibility,

$$\chi = \frac{\partial m}{\partial h} = \frac{\partial}{\partial h}\left(\frac{1}{2} - C_0\sqrt{h_{c2} - h}\right) = \frac{C_0}{2\sqrt{h_{c2} - h}}. \tag{4.78}$$

The double occupancy density ω for a given density $n_{i\downarrow}$ in the limit $n_{i\downarrow} \to 0$ is given by

$$\begin{aligned}\omega = \frac{1}{L}\frac{\partial E}{\partial U} &= \left(1 - \frac{U/4}{\sqrt{1+(U/4)^2}}\right) n_{i\downarrow} + \frac{\pi^2}{24}\frac{U}{\left(1+(U/4)^2\right)^{\frac{3}{2}}} n_{i\downarrow}^3 \\ &\approx \left(1 - \frac{U/4}{\sqrt{1+(U/4)^2}}\right) n_{i\downarrow} = C_1 n_{i\downarrow}. \end{aligned} \tag{4.79}$$

We can now calculate the entanglement parameters as a function of the magnetic field:

$$u^+ = 1 - n_{i\downarrow} - \omega = 1 - \left(2 - \frac{U/4}{\sqrt{1+(U/4)^2}}\right) n_{i\downarrow} = 1 - C_2 n_{i\downarrow} \tag{4.80}$$

$$u^- = n_{i\downarrow} - \omega = \left(\frac{U/4}{\sqrt{1+(U/4)^2}}\right) n_{i\downarrow} = C_3 n_{i\downarrow} \tag{4.81}$$

$$z = \omega. \tag{4.82}$$

This yields for the entanglement:

$$\begin{aligned} E_\nu(h) &= -\left(2C_1 n_{i\downarrow}(h)\right)\log_2\left(C_1 n_{i\downarrow}(h)\right) - \left(1 - C_2 n_{i\downarrow}(h)\right)\log_2\left(1 - C_2 n_{i\downarrow}(h)\right) \\ &- \left(C_3 n_{i\downarrow}(h)\right)\log_2\left(C_3 n_{i\downarrow}(h)\right). \end{aligned} \tag{4.83}$$

Taking the derivative of the entanglement in the critical region $h \to h_{c2}$, we obtain

$$\begin{aligned}\frac{dE_\nu}{dh} &= -\left(2C_1\frac{dn_{i\downarrow}}{dh}\right)\log_2\left(C_1 n_{i\downarrow}(h)\right) + \left(C_2\frac{dn_{i\downarrow}(h)}{dh}\right)\log_2\left(1 - C_2 n_{i\downarrow}(h)\right) \\ &- \left(C_3\frac{dn_{i\downarrow}(h)}{dh}\right)\log_2\left(C_3 n_{i\downarrow}(h)\right), \end{aligned} \tag{4.84}$$

with

$$\frac{dn_{i\downarrow}}{dh} = -\frac{dm}{dh} = -\chi. \tag{4.85}$$

This means that we can rewrite the derivative as

$$\begin{aligned}\frac{dE_\nu}{dh} &= \left(2C_1\chi\right)\log_2\left(C_1 n_{i\downarrow}(h)\right) - \left(C_2\chi\right)\log_2\left(1 - C_2 n_{i\downarrow}(h)\right) \\ &+ \left(C_3\chi\right)\log_2\left(C_3 n_{i\downarrow}(h)\right). \end{aligned} \tag{4.86}$$

When we get close to the critical field h_{c2} the dominating terms in eqn. (4.84) will be

$$\begin{aligned}\frac{\partial E_\nu}{\partial h} &\simeq \left(2C_1\chi\right)\log_2\left(C_1 C_0\sqrt{h_{c2}-h}\right) + \left(C_3\chi\right)\log_2\left(C_3 C_0\sqrt{h_{c2}-h}\right) \\ &= \chi\left(\frac{2C_1 + C_3}{2\ln(2)}\right)\left(\ln(h_{c2}-h) + \text{const.}\right). \end{aligned} \tag{4.87}$$

4.6 Away from half-filling

In this section we will study the effect of a chemical potential in the repulsive case in an open system. We make the simplifying assumption that the environment acts solely as a particle reservoir at T=0 and does not influence the dynamics. When we add the chemical potential to the Hubbard Hamiltonian it takes the form

$$H = -t\sum_{i=1}^{L}(\hat{c}_{ia}^{\dagger}\hat{c}_{i+1a} + h.c.) + U\sum_{i=1}^{L}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} - \mu\sum_{i=1}^{L}(\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}). \tag{4.88}$$

For simplicity we have set the magnetic field to zero.The last term will control the number of particles in our system since if μ is negative we have to pay a price in energy for each added particle. We start by focusing on what we can use from our previous analysis. The double occupancy can still be expressed as the derivative of the ground state energy:

$$\omega = \frac{1}{L}\frac{\partial E_0}{\partial U}. \tag{4.89}$$

The Lieb-Mattis theorem [35] tells us that the ground state will still be a singlet independently of the particle concentration. This means that the parameters for spin up, spin down and zero occupation are given by

$$u^{+} = \langle\hat{n}_{\uparrow}\rangle = \frac{n}{2} - \omega \tag{4.90}$$

$$u^{-} = \langle\hat{n}_{\downarrow}\rangle = \frac{n}{2} - \omega \tag{4.91}$$

$$z = 1 - u^{+} - u^{-} - \omega = 1 - n + \omega. \tag{4.92}$$

In the previous chapter we found a series expansion for the ground state energy per site for $U \gg 1$, given by the expression

$$\frac{E}{L} = -\frac{2}{\pi}\sin(\pi n) - \sum_{l=1}^{\infty}\kappa_l(n)\left(\frac{1}{U}\right)^{l}. \tag{4.93}$$

Now eqns. (4.89) and (4.93) implies that doubly occupied states are given by

$$\omega = \frac{1}{L}\frac{\partial E}{\partial U} = \sum_{l=1}^{\infty} l\kappa_l(n)\left(\frac{1}{U}\right)^{l+1}. \tag{4.94}$$

Here $\kappa_l(n)$ is given in tab. (3.1). In the limit $U \to 0$ we have from [27] that

$$\omega = \frac{n^2}{4}. \tag{4.95}$$

We are now in a position where we can plot the entanglement versus fillingfactor in the Hubbard model. This is done in fig. (4.4). The next step is to try to find the relation between n and μ, since it is more natural to study the effect of a change in μ (which is experimentally controllable) rather than a change in the particle density. We can again use the Hellman-Feynman theorem and take the derivative of the ground state energy, but this time w.r.t. n. This will give us μ:

$$\mu = \frac{1}{L}\frac{\partial E}{\partial n}. \tag{4.96}$$

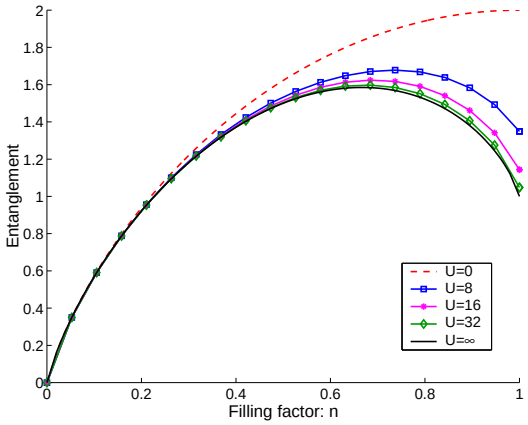


Figure 4.4: Local entanglement versus filling factor n.

From linkngroundE we see that when $U \to \infty$ we can find an analytical relation between n and μ which is invertible in the region $0 < n < 1$:

$$\mu = \frac{1}{L}\frac{\partial E}{\partial n} = -2\cos(\pi n), \tag{4.97}$$

with inverse

$$n(\mu) = \frac{1}{\pi}\arccos\left(-\frac{\mu}{2}\right). \tag{4.98}$$

In the limit $U \to 0$ we have from [36] that the relation between μ and n is

$$\mu = -2\cos\left(\frac{n\pi}{2}\right). \tag{4.99}$$

This gives

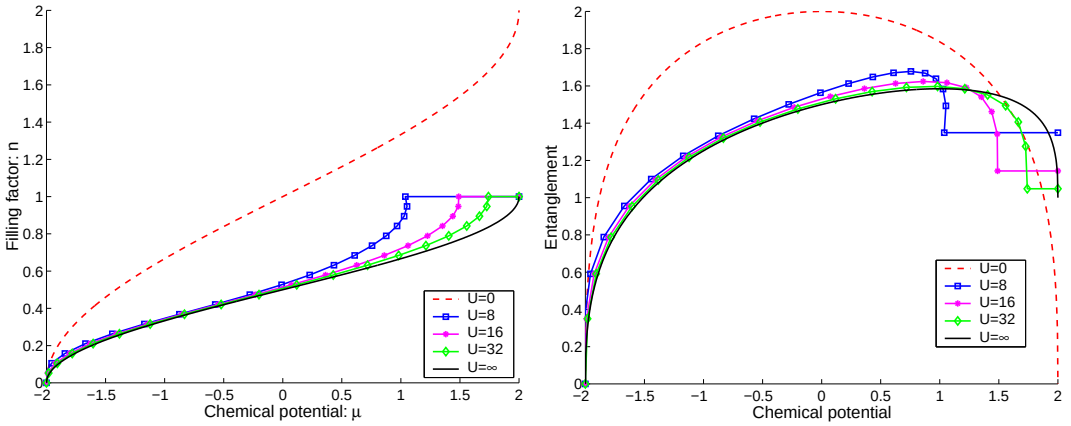
$$n(\mu) = \frac{2}{\pi}\arccos\left(-\frac{\mu}{2}\right). \tag{4.100}$$

We can now calculate the chemical potential as a function of n for the case when $4 < U < \infty$ by use of the series expansion from [27]:

$$\mu(n) = \frac{\partial E}{\partial n} = -2\cos(\pi n) - \sum_{l=1}^{\infty}\left(\frac{\partial}{\partial n}\kappa_l(n)\right)\left(\frac{1}{U}\right)^l. \tag{4.101}$$

In the region $0 < n < 1$ we can invert $\mu(n)$ analytically and find n as a function of μ in the limits $U = 0+$ and $U = \infty$. In the interval $4 < U < \infty$ we can plot $n(\mu)$ numerically by calculating $\mu(n)$ and plotting it against the corresponding n; this is done in fig. (4.5(a)). In the same way we can use both our exact result and numerical result to plot $E_\nu(\mu)$ for a number of different values of U. All this is done in fig. (**??**) We now see that the entanglement has a more violent behavior at the critical point, as compared to E_ν as a function of n. We investigate the derivative of the entanglement in the same way as earlier in this chapter. For the case $U = \infty$ we obtain the following behavior at $\mu \to \mu_{c1}$:

$$\begin{aligned}\frac{\partial E_\nu}{\partial \mu} &= -\chi_{c1}\left(\log_2\left(\frac{1}{2\pi}\sqrt{\mu - \mu_{c1}}\right)\right) \\ &= -C\chi_{c1}(\ln(\mu - \mu_{c1}) + \text{const.}).\end{aligned} \tag{4.102}$$



(a) Filling factor vs chemical potential. (b) Entanglement vs chemical potential.

Figure 4.5:

In the limit $\mu \to \mu_{c2}$ we have

$$\frac{\partial E_\nu}{\partial \mu} = -\chi_{c2}\left(\log_2\left(\frac{1}{\pi}\sqrt{\mu_{c2}-\mu)}\right)\right) \tag{4.103}$$

$$= -C\chi_{c2}\left(\ln(\mu_{c2}-\mu)+\text{const.}\right). \tag{4.104}$$

In both cases $C = 1/(2\ln(2))$ while

$$\chi_{c1} = \left.\frac{\partial n}{\partial \mu}\right|_{\mu=\mu_{c1}} = \frac{1}{2\pi\sqrt{\mu-\mu_{c1}}} \tag{4.105}$$

$$\chi_{c2} = \left.\frac{\partial n}{\partial \mu}\right|_{\mu=\mu_{c2}} = \frac{1}{2\pi\sqrt{\mu_{c2}-\mu}}. \tag{4.106}$$

In the case when $U = 0^+$ we obtain the following behavior at $\mu \to \mu_{c1}$:

$$\frac{\partial E_\nu}{\partial \mu} = -\chi\left(\log_2\left(\frac{1}{\sqrt{2}\pi}\sqrt{\mu-\mu_{c1}}\right)\right) \tag{4.107}$$

$$= -C\chi\ln\left(\frac{1}{2\pi^2}(\mu-\mu_{c1})\right) = \tag{4.108}$$

$$= -C\chi\left(\ln(\mu-\mu_{c1})+\text{const.}\right), \tag{4.109}$$

where

$$\chi = \left.\frac{\partial n}{\partial \mu}\right|_{\mu=\mu_{c1}} = \frac{1}{\pi\sqrt{\mu-\mu_{c1}}}. \tag{4.110}$$

We see that the derivative of the entanglement at the critical point is once again divergent and that the behavior at the critical point is the same as for the attractive case with a magnetic field. That this is not a coincidence will be shown in the next chapter by the use of a particle-hole transformation. But now we turn our attention to the case $8 \leq U < \infty$. We expect that the derivative of the entanglement will behave as

$$\frac{\partial E_\nu}{\partial \mu} = C\chi \tag{4.111}$$

at the critical point μ_{c2}. The reason for this is that the logarithmic divergence now dissapears since we have a mixture of all four states at the critical point μ_{c2}. We have from eqn. (4.90) and eqn. (4.91) that $u^+ = u^- = n/2 - \omega$. From eqn. (4.92) we have $z = 1 - n + \omega$ and finally from eqn. (4.94) we have

$$\omega = \sum_{l=1}^{\infty} l\kappa_l(n) \left(\frac{1}{U}\right)^{l+1}. \tag{4.112}$$

This adds up to the following form for the entanglement:

$$E_\nu(n) = -(n-2\omega)\log_2(n/2-\omega) - (1-n+\omega)\log_2(1-n+\omega) - \omega\log_2\omega. \tag{4.113}$$

If we now take the derivative of eqn. (4.113) w.r.t. μ we obtain

$$\begin{aligned}
\frac{\partial E_\nu(n)}{\partial\mu} &= -\left(\frac{\partial n}{\partial\mu} - 2\frac{\partial\omega}{\partial\mu}\right)\log_2 u^+ \\
&+ \left(\frac{\partial n}{\partial\mu} - \frac{\partial\omega}{\partial\mu}\right)\log_2 z - \frac{\partial\omega}{\partial\mu}\log_2\omega \\
&= -\frac{\partial n}{\partial\mu}\left(\log_2 u^+ - \log_2 z\right) \\
&+ \frac{\partial\omega}{\partial\mu}\left(2\log_2 u^+ - \log_2 z - \log_2\omega\right).
\end{aligned} \tag{4.114}$$

Since we have assumed that $8 \leq U$ we know that $z, \omega < u^+$ and in the limit $n \to 1$ we also have that $z \to \omega$. This implies that $\log_2 z$ and $\log_2\omega$ will dominate over $\log_2 u^+$. We then obtain

$$\frac{\partial E_\nu(n)}{\partial\mu} \approx \frac{\partial n}{\partial\mu}\log_2 z - \frac{\partial\omega}{\partial\mu}\left(\log_2 z + \log_2\omega\right). \tag{4.115}$$

It is now time to study $\partial\omega/\partial\mu$ and to do this we use the series expansion from [27]:

$$\frac{\partial\omega}{\partial\mu} = \sum_{l=1}^{\infty} l\left(\frac{1}{U}\right)^{l+1}\frac{\partial\kappa_l(n)}{\partial\mu}. \tag{4.116}$$

In this expansion we have explicit expressions for first five terms in $\kappa_l(n)$ [27], and using the chain rule to find the derivative we obtain in the limit $n \to 1$:

$$\frac{\partial\omega}{\partial\mu} \approx \frac{\partial n}{\partial\mu}\left(\frac{4\ln 2}{U^2} - \frac{45\zeta(3)}{U^4} + \frac{1425\zeta(5)}{2U^6}\right). \tag{4.117}$$

When $8 \leq U$ we have

$$\frac{\partial\omega}{\partial\mu} \leq 0.0329\frac{\partial n}{\partial\mu}. \tag{4.118}$$

Using eqn. (4.118) we can approximate eqn. (4.115) by

$$\frac{\partial E_\nu}{\partial\mu} \sim \frac{\partial n}{\partial\mu}\log_2(z). \tag{4.119}$$

When $8 \leq U < \infty$ we have that $0 < z < 1$ which means that $\log_2 z < 0$. We define $|\log_2(z)| = C < \infty$ and thus obtain

$$\frac{\partial E_\nu}{\partial \mu} \sim -C\frac{\partial n}{\partial \mu} = -C\chi. \tag{4.120}$$

In [9] the derivative of $E_\nu(n)$ w.r.t. n is calculated so why should we go through all this trouble just to calculate it w.r.t. μ instead? The answer is simply because μ is the experimentally accessible parameter. That this is important can easily be seen be comparing fig. (**??**) and fig. (4.4). In fig. (4.4) we see no sign of the divergences that we find at the QPT points. This is also the probable reason why this signature of a second order QPT was missed in ref. [9] (where instead the derivative of E_ν w.r.t. n was calculated). In ref. [9] the following relation is found:

$$\left.\frac{dE_\nu}{dn}\right|_{n=1^-} = -\left.\frac{dE_\nu}{dn}\right|_{n=1^+}. \tag{4.121}$$

This relation can easily be seen to follow from $E_\nu(n) = E_\nu(2-n)$ which will be proven in the next chapter by a particle-hole transformation. The logic in ref. [**?**], where critical behaviour is inferred from the discontinuity of the derivatives at $n = 1^+$ and $n = 1^-$, is somewhat strange. In fact, the two points are widely separated if $U > 0$, which has been known since the first Bethe ansatz solution in 1968 [22]. This can be stated as $\mu_- < \mu_+$ where μ_-/μ_+ is the chemical potential needed to remove/add one particle at half-filling. So if two points are widely separated it is no surprise that the derivative at these two points are different. Therefore their difference can not be considered as a sign of criticality. If one studies entanglement as a function of chemical potential we obtain a divergent behavior, as predicted in [8], and which characterizes a second order QPT.

Chapter 5

Particle-hole transformations

A smart way to calculate things is to use known results and apply a transformation that extends them to a new regime, or to a new model. One such smart trick is to use particle-hole transformations. These transformations will be introduced in this chapter and used to extend the results in the previous chapter into new regions.

5.1 Particle-hole transformation: an introduction

We start from the Hubbard Hamiltonian with magnetic field and chemical potential:

$$\begin{aligned} H &= -t\sum_{i=1}^{L}(\hat{c}_{ia}^{\dagger}\hat{c}_{i+1a} + h.c.) + U\sum_{i=1}^{L}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} - \mu\sum_{i=1}^{L}(\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}) \\ &- \frac{h}{2}\sum_{i=1}^{L}(\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow}). \end{aligned} \tag{5.1}$$

Given this Hamiltonian we perform the following transformations:

$$\hat{a}_{i\downarrow}^{\dagger} = (-1)^i\hat{c}_{i\downarrow} \qquad \hat{a}_{i\downarrow} = (-1)^i\hat{c}_{i\downarrow}^{\dagger} \tag{5.2}$$

$$\hat{a}_{i\uparrow}^{\dagger} = (-1)^i\hat{c}_{i\uparrow} \qquad \hat{a}_{i\uparrow} = (-1)^i\hat{c}_{i\uparrow}^{\dagger}. \tag{5.3}$$

This transformation is called a particle-hole transformation. The reason for this can be realized by studying what it does: The creation operator $\hat{a}_{i\uparrow}^{\dagger}$ kills a particle with spin up at site i and creates a hole. In the same way the destruction operator $\hat{a}_{i\uparrow}$ destroys a hole by creating a particle. So by a particle-hole transformation particles are exchanged for holes and vice versa. If we insert the transformation in eqns. (5.2) and (5.3) into the Hamiltonian in eqn. (5.1) we get

$$\begin{aligned} H' &= -t\sum_{i=1}^{L}(-\hat{a}_{i+1\uparrow}\hat{a}_{i\uparrow}^{\dagger} - \hat{a}_{i\uparrow}\hat{a}_{i+1\uparrow}^{\dagger} - \hat{a}_{i\downarrow}\hat{a}_{i+1\downarrow}^{\dagger} - \hat{a}_{i+1\downarrow}\hat{a}_{i\downarrow}^{\dagger}) \\ &+ U\sum_{i=1}^{L}\hat{a}_{i\uparrow}\hat{a}_{i\uparrow}^{\dagger}\hat{a}_{i\downarrow}\hat{a}_{i\downarrow}^{\dagger} - \mu\sum_{i=1}^{L}(\hat{a}_{i\uparrow}\hat{a}_{i\uparrow}^{\dagger} + \hat{a}_{i\downarrow}\hat{a}_{i\downarrow}^{\dagger}) \\ &- \frac{h}{2}\sum_{i=1}^{L}(\hat{a}_{i\uparrow}\hat{a}_{i\uparrow}^{\dagger} - \hat{a}_{i\downarrow}\hat{a}_{i\downarrow}^{\dagger}). \end{aligned} \tag{5.4}$$

The particle-hole transformation in eqns. (5.2) and (5.3) is canonical and the new operators hence satisfy the usual anti-commutation relations

$$\{\hat{a}_{i\sigma}, \hat{a}_{i\sigma'}\} = \{\hat{a}^\dagger_{i\sigma}, \hat{a}^\dagger_{i\sigma'}\} = 0 \qquad \{\hat{a}^\dagger_{i\sigma}, \hat{a}_{i\sigma'}\} = \delta_{ii'}\delta_{\sigma\sigma'}. \tag{5.5}$$

If we use these relations we can write the transformed Hamiltonian as

$$\begin{aligned} H' &= -t\sum_{i=1}^{L}(\hat{a}^\dagger_{i\uparrow}\hat{a}_{i+1\uparrow} + \hat{a}^\dagger_{i+1\uparrow}\hat{a}_{i\uparrow} + \hat{a}^\dagger_{i+1\downarrow}\hat{a}_{i\downarrow} + \hat{a}^\dagger_{i\downarrow}\hat{a}_{i+1\downarrow}) + L(U-2\mu) \\ &+ U\sum_{i=1}^{L}\hat{a}^\dagger_{i\uparrow}\hat{a}_{i\uparrow}\hat{a}^\dagger_{i\downarrow}\hat{a}_{i\downarrow} - (U-\mu)\sum_{i=1}^{L}(\hat{a}^\dagger_{i\uparrow}\hat{a}_{i\uparrow} + \hat{a}^\dagger_{i\downarrow}\hat{a}_{i\downarrow}) \\ &+ \frac{h}{2}\sum_{i=1}^{L}(\hat{a}^\dagger_{i\uparrow}\hat{a}_{i\uparrow} - \hat{a}^\dagger_{i\downarrow}\hat{a}_{i\downarrow}). \end{aligned} \tag{5.6}$$

The particle-hole transformation changes the particle numbers as

$$N_\uparrow \to L - N_\uparrow \qquad N_\downarrow \to L - N_\downarrow. \tag{5.7}$$

This has the effect that if we are in a less than half-filled band ($n < 1$) we get the more than half-filled band ($n < 1$) after the transformation. This means that we can find the quantum critical points in the more than half-filled case by first identifying the ones in the less than half-filled case. The quantum critical point where we go from half-filling to more than half-filling corresponds to $\mu_{c3} = U - \mu_{c2}$ and the point where we have $N = 2L$ (completely filled band) corresponds to $\mu_{c4} = U - \mu_{c1}$. Let us now return to the study of entanglement and the effect that the particle-hole transformation eqns. (5.2) and (5.2) has on the entanglement parameters in the system:

$$u^+ \to u^- \qquad u^- \to u^+ \tag{5.8}$$

$$z \to \omega \qquad \omega \to z. \tag{5.9}$$

This means that if we know the entanglement for the less than half-filled *or* more than half-filled case we can calculate the other case from the following formula:

$$E_\nu(n) = E_\nu(2-n). \tag{5.10}$$

In the same way we have that

$$E_\nu(h) = E_\nu(-h). \tag{5.11}$$

5.2 Filling versus magnetization

We once again start from the Hubbard model with a chemical potential μ and a magnetic field h:

$$\begin{aligned} H &= -t\sum_{i=1}^{L}(\hat{c}^\dagger_{ia}\hat{c}_{i+1a} + h.c.) + U\sum_{i=1}^{L}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} - \mu\sum_{i=1}^{L}(\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}) \\ &- \frac{h}{2}\sum_{i=1}^{L}(\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow}). \end{aligned} \tag{5.12}$$

But now we perform another transformation:

$$\hat{a}^\dagger_{i\uparrow} = (-1)^i \hat{c}_{i\uparrow} \qquad \hat{a}_{i\uparrow} = (-1)^i \hat{c}^\dagger_{i\uparrow}. \tag{5.13}$$

This transforms the Hamiltonian in eqn. (5.12) into

$$\begin{aligned} H' &= -t\sum_{i=1}^{L}(-\hat{a}_{i\uparrow}\hat{a}^\dagger_{i+1\uparrow} - \hat{a}_{i+1\uparrow}\hat{a}^\dagger_{i\uparrow} + \hat{c}^\dagger_{i\downarrow}\hat{c}_{i+1\downarrow}\hat{c}^\dagger_{i\downarrow}\hat{c}_{i+1\downarrow}) \\ &+ U\sum_{i=1}^{L}\hat{a}_{i\uparrow}\hat{a}^\dagger_{i\uparrow}\hat{c}^\dagger_{i\downarrow}\hat{c}_{i\downarrow} - \mu\sum_{i=1}^{L}(\hat{a}_{i\uparrow}\hat{a}^\dagger_{i\uparrow} + \hat{c}^\dagger_{i\downarrow}\hat{c}_{i\downarrow}) \\ &- \frac{h}{2}\sum_{i=1}^{L}(\hat{a}_{i\uparrow}\hat{a}^\dagger_{i\uparrow} - \hat{c}^\dagger_{i\downarrow}\hat{c}_{i\downarrow}). \end{aligned} \tag{5.14}$$

If we use the anti commutation relations from eqn. (5.5) we can rewrite this as

$$\begin{aligned} H' &= -t\sum_{i=1}^{L}(\hat{a}^\dagger_{i\uparrow}\hat{a}_{i+1\uparrow} + \hat{a}^\dagger_{i+1\uparrow}\hat{a}_{i\uparrow} + \hat{c}^\dagger_{i\downarrow}\hat{c}_{i+1\downarrow}\hat{c}^\dagger_{i\downarrow}\hat{c}_{i+1\downarrow}) \\ &- U\sum_{i=1}^{L}\hat{a}^\dagger_{i\uparrow}\hat{a}_{i\uparrow}\hat{c}^\dagger_{i\downarrow}\hat{c}_{i\downarrow} - \left(\frac{U}{2} - \mu\right)\sum_{i=1}^{L}(\hat{a}^\dagger_{i\uparrow}\hat{a}_{i\uparrow} - \hat{c}^\dagger_{i\downarrow}\hat{c}_{i\downarrow}) \\ &+ \left(\frac{U}{2} + \frac{h}{2}\right)\sum_{i=1}^{L}(\hat{a}^\dagger_{i\uparrow}\hat{a}_{i\uparrow} + \hat{c}^\dagger_{i\downarrow}\hat{c}_{i\downarrow}). \end{aligned} \tag{5.15}$$

The transformation in eqn. (5.13) implies for the particle numbers:

$$N_\uparrow \to L - N_\uparrow \qquad N_\downarrow \to N_\downarrow. \tag{5.16}$$

This means that the less than half-filled case with no magnetic-field transforms to the case of positive magnetic-field at half-filling, and the more than half-filled case transforms to the case when we have a negative magnetization since after transformation we have that $\sum_{i=1}^{L}(n_{i\uparrow} - n_{i\downarrow})/L = 2m = 1 - n$. This implies that the chemical potential now plays the role of a magnetic field. We can now find the critical points for the magnetic field where the first spin flips, $h = h_{c1}$, and where we obtain full magnetization, $h = h_{c2}$. For comparison, let us start by writing down the Hubbard model with a magnetic field:

$$H = -t\sum_{i=1}^{L}(\hat{c}^\dagger_{ia}\hat{c}_{i+1a} + h.c.) + U\sum_{i=1}^{L}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} - \frac{h}{2}\sum_{i=1}^{L}(\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow}). \tag{5.17}$$

Comparing eqns. (5.15) and 5.17 we see that the magnetic field in eqn. (5.17) has the magnitude $h = 2(U/2 - \mu)$. This implies that we can find our two critical points for positive magnetization. The case when $n = 0$ corresponds to $m = 1/2$ and this in turn corresponds to $\mu = \mu_{c1}$. This gives us the following relation for the critical field h_{c1}:

$$h_{c1} = 2\left(\frac{U}{2} - \mu_{c1}\right) = U - 2\mu_{c1}. \tag{5.18}$$

In the same way $n = 1$ correspond to m=0 which implies:

$$h_{c2} = 2\left(\frac{U}{2} - \mu_{c2}\right) = U - 2\mu_{c2}. \tag{5.19}$$

Similarly we have that h_{c3} $(m = 0)$ and h_{c4} $(m = -1/2)$ are given by

$$h_{c3} = 2\left(\frac{U}{2} - \mu_{c3}\right) = 2(U/2 - U + \mu_{c2}) = -U + 2\mu_{c2} \tag{5.20}$$

$$h_{c4} = 2\left(\frac{U}{2} - \mu_{c4}\right) = 2(U/2 - U + \mu_{c1}) = -U + 2\mu_{c1}. \tag{5.21}$$

When we transform from the repulsive Hubbard model with chemical potential to the attractive Hubbard model with magnetic field the entanglement parameters transform as follows when $0 \leq n \leq 1$:

$$z \to u^+ \qquad u^+ \to z \tag{5.22}$$

$$\omega \to u^- \qquad u^- \to \omega. \tag{5.23}$$

When $1 \leq n \leq 2$ we have instead

$$z \to u^- \qquad u^- \to z \tag{5.24}$$

$$\omega \to u^+ \qquad u^+ \to \omega. \tag{5.25}$$

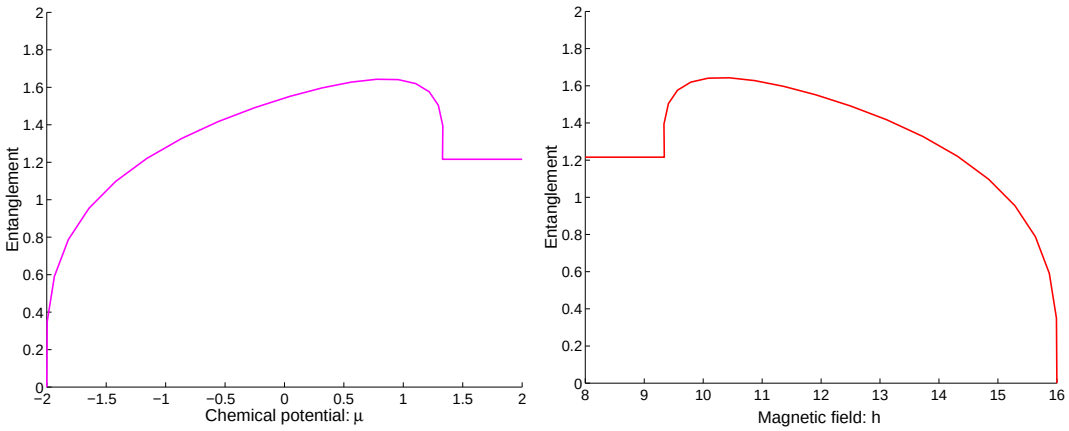
5.3 The use of particle-hole transformations

To give the reader a feeling for what a powerful tool the particle-hole transformation is we will here discuss the cases we have calculated and what other information can be extracted. We started with the attractive Hubbard model with a magnetic field $h \geq 0$ in the $U \to 0$ or $U \to -\infty$ limits. This can be transformed by eqns. (5.2) and (5.3) into the case when $h < 0$. If we use eqn. (5.13) instead we can transform the attractive Hubbard model with magnetic field for $-\infty \leq h \leq \infty$ into the repulsive model with chemical potential for $-\infty \leq \mu \leq \infty$. In the same way we can by the same particle-hole transformation eqn. (5.13) transform from the repulsive to the attractive case. We can also use eqns. (5.2) and (5.3) to investigate how the entanglement behaves in the region where $1 < n < 2$ from our knowledge about $0 < n < 1$. To give an example: We can transform the repulsive Hubbard with chemical potential and finite U fig. (5.1(a)) into the attractive case with magnetic field and finite U fig. (5.1(b)) by the particle-hole transformation

$$\hat{c}^\dagger_{i\uparrow} = (-1)^i \hat{a}_{i\uparrow} \tag{5.26}$$

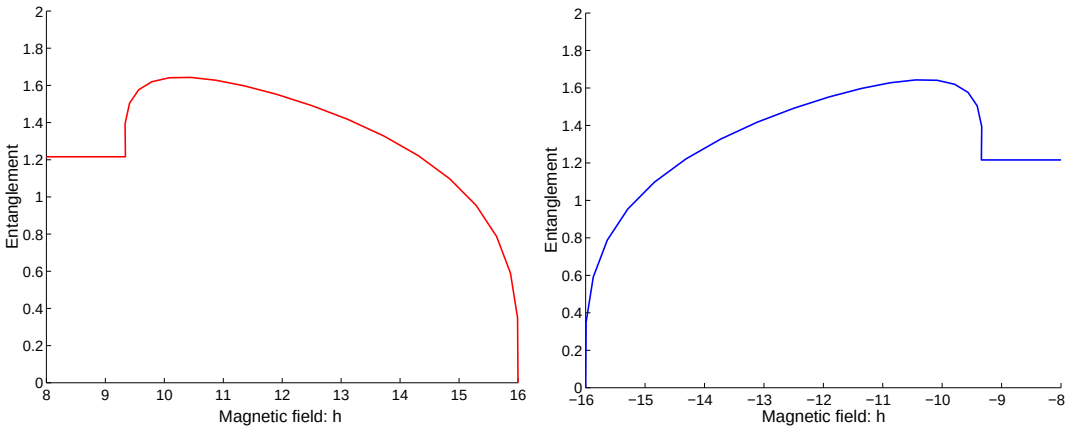
$$\hat{c}_{i\uparrow} = (-1)^i \hat{a}^\dagger_{i\uparrow}. \tag{5.27}$$

This transformation takes $N_\uparrow \to L - N_\uparrow$ and the chemical potential takes the the role of a magnetic field $\mu \to h(\mu) = |U| - \mu$. We can write the relation between the entanglement in the attractive and repulsive cases as $E(h(\mu)) = E(\mu)$. This implies that $E(\mu_{c1}) = E(h_{c2})$ and $E(\mu_{c2}) = E(h_{c1})$. We can then use eqns. (5.2) and (5.3) to transform the attractive case with a magnetic field $h > 0$ fig. (5.2(a)) into the attractive case with a magnetic field $h < 0$ linkfigspridning5.



(a) Entanglement vs chemical potential ($U = 12$). (b) Entanglement vs magnetic field ($U = -12$).

Figure 5.1: Particle-hole transformation



(a) Entanglement vs magnetic field ($U = -12$). (b) Entanglement vs magnetic field ($U = -12$).

Figure 5.2: Particle-hole transformation

Chapter 6

Concluding remarks

The aim of this thesis was to study the relation between entanglement and quantum phase transitions. So we started with the simplest case of an interacting electron system that exhibits a quantum phase transition (QPT): a hopping term and an on-site interaction (alias the Hubbard model in it's simplest form). This model exhibits a Mott transition at $U = 0$ and at this point we found that the entanglement as measured by the von Neumann entropy has a maximum. So at this stage our work were in agreement with one of the first conjectures that entanglement is maximal at the QPT point. But this conjecture ran into problems already if we add a chemical potential, so as to model the situation with a system connected to a particle reservoir. This new model has a maximum away from the QPT points defining the transitions to empty and half-filled lattices, respectively.

The next step in our study was related to the work [7] and [8]. Here the derivative of the concurrence was studied and in [8] it was conjectured that a 2:nd order QPT has a divergence in the first derivative of the concurrence at the critical point. The relation between concurrence and the von Neumann entropy for a system of iterant electrons is still an open question. In the Hubbard model we can obtain a 2:nd order phase transition if we add a chemical potential or a magnetic field. For the attractive Hubbard model with a magnetic field we found that at the critical points in the large-U and weak-U limits the derivative of the entanglement scales as

$$\frac{\partial E_\nu}{\partial h} = \pm C\chi \ln(|h - h_c|). \tag{6.1}$$

The fact that an entanglement measure of a critical many-particle system can be *quantitatively* linked to a physical observable is a striking result and goes beyond standard constructions of entanglement witnesses [39] that merely detect the presence of entanglement. To find a physical interpretation of the results, and to explore whether it can be extended to other critical quantum many-particle system, is a challenging and fascinating problem.

Appendix A

Some algebraic relations

In this appendix we will show that $B(\beta_1)B(\beta_2)|\omega\rangle$ is an eigenstate to $Z(\alpha) = A(\alpha) + D(\alpha)$ except for some unwanted terms that can be made to vanish provided that a certain condition is fulfilled. (For definitions of the operators A,B,D and the state $|\omega\rangle$ see sect. (3.4).) To be able to show this we need the following algebraic relations

$$\begin{array}{l} A(\alpha)B(\beta) = u(\beta-\alpha)B(\beta)A(\alpha) + v(\beta-\alpha)B(\alpha)A(\beta) \\ D(\alpha)B(\beta) = u(\alpha-\beta)B(\beta)A(\alpha) + v(\alpha-\beta)B(\alpha)A(\beta) \end{array} , \tag{A.1}$$

with

$$\begin{array}{lll} u(\alpha) & = \frac{1}{a(\alpha)} & = \frac{\alpha+ic}{\alpha} \\ v(\alpha) & = -\frac{b(\alpha)}{a(\alpha)} & = -\frac{ic}{\alpha} \end{array} . \tag{A.2}$$

Furthermore

$$\begin{array}{l} A(\alpha)A(\beta) = A(\beta)A(\alpha) \\ B(\alpha)B(\beta) = B(\beta)B(\alpha) \\ D(\alpha)D(\beta) = D(\beta)D(\alpha). \end{array} \tag{A.3}$$

We shall start by using the following condition, obtained from the Yang-Baxter relation:

$$R(\Xi(\alpha)\otimes\Xi(\beta)) = (\Xi(\beta)\otimes\Xi(\alpha))R. \tag{A.4}$$

We can rewrite this in explicit form using the short-hand notation $A_\alpha = A(\alpha)$, $a = a(\alpha-\beta)$, ... where we have suppressed the arguments:

$$\begin{array}{l} \left(\begin{array}{cccc} A_\alpha A_\beta & A_\alpha B_\beta & B_\alpha A_\beta & B_\alpha B_\beta \\ bA_\alpha C_\beta + aC_\alpha A_\beta & bA_\alpha D_\beta + aC_\alpha B_\beta & bB_\alpha C_\beta + aD_\alpha A_\beta & bB_\alpha D_\beta + aD_\alpha B_\beta \\ aA_\alpha C_\beta + bC_\alpha A_\beta & aA_\alpha D_\beta + bC_\alpha B_\beta & aB_\alpha C_\beta + bD_\alpha A_\beta & aB_\alpha D_\beta + bD_\alpha B_\beta \\ C_\alpha C_\beta & C_\alpha D_\beta & D_\alpha C_\beta & D_\alpha D_\beta \end{array}\right) \\ = \left(\begin{array}{cccc} A_\beta A_\alpha & bA_\beta B_\alpha + aB_\beta A_\alpha & aA_\beta B_\alpha + bB_\beta A_\alpha & B_\beta B_\alpha \\ A_\beta C_\alpha & bA_\beta D_\alpha + aB_\beta C_\alpha & aA_\beta D_\alpha + aB_\beta C_\alpha & B_\beta D_\alpha \\ C_\beta A_\alpha & bC_\beta B_\alpha + aD_\beta A_\alpha & aC_\beta B_\alpha + bD_\beta A_\alpha & D_\beta B_\alpha \\ C_\beta C_\alpha & bC_\beta D_\alpha + aD_\beta C_\alpha & aC_\beta D_\alpha + bD_\beta C_\alpha & D_\beta D_\alpha \end{array}\right). \end{array} \tag{A.5}$$

From this relation we easily see that eqn. (A.3) is fulfilled. What is left to do is to prove eqn. (A.1). To do this we note that

$$A(\alpha)B(\beta) = b(\alpha-\beta)A(\beta)B(\alpha) + a(\alpha-\beta)B(\beta)A(\alpha) \tag{A.6}$$

$$B(\alpha)A(\beta) = a(\alpha-\beta)A(\beta)B(\alpha) + b(\alpha-\beta)B(\beta)A(\alpha). \tag{A.7}$$

Now we multiply eqn. (A.7) by b/a and then subtract the resulting equations from eqn. (A.6)

$$A(\alpha)B(\beta) - \frac{b(\alpha-\beta)}{a(\alpha-\beta)}B(\alpha)A(\beta) \quad = \quad \left(a(\alpha-\beta) - \frac{b^2(\alpha-\beta)}{a(\alpha-\beta)}\right)B(\beta)A(\alpha). \tag{A.8}$$

This we can rearrange to

$$A(\alpha)B(\beta) \quad = \quad \left(a(\alpha-\beta) - \frac{b^2(\alpha-\beta)}{a(\alpha-\beta)}\right)B(\beta)A(\alpha) + \frac{b(\alpha-\beta)}{a(\alpha-\beta)}B(\alpha)A(\beta). \tag{A.9}$$

A simple calculation now shows that

$$a(\alpha-\beta) - \frac{b^2(\alpha-\beta)}{a(\alpha-\beta)} = \frac{1}{a(\beta-\alpha)} = u(\beta-\alpha) \tag{A.10}$$

$$\frac{b(\alpha-\beta)}{a(\alpha-\beta)} = -\frac{b(\beta-\alpha)}{a(\beta-\alpha)} = v(\beta-\alpha). \tag{A.11}$$

Hence

$$A(\alpha)B(\beta) = u(\beta-\alpha)B(\beta)A(\alpha) + v(\beta-\alpha)B(\alpha)A(\beta). \tag{A.12}$$

Finally we note that

$$b(\alpha-\beta)B(\alpha)D(\beta) + a(\alpha-\beta)D(\alpha)B(\beta) = B(\beta)D(\alpha), \tag{A.13}$$

which can be rewritten as

$$D(\alpha)B(\beta) = \frac{-b(\alpha-\beta)}{a(\alpha-\beta)}B(\alpha)D(\beta) + \frac{1}{a(\alpha-\beta)}B(\beta)D(\alpha) \tag{A.14}$$

i.e.

$$D(\alpha)B(\beta) = u(\alpha-\beta)B(\beta)A(\alpha) + v(\alpha-\beta)B(\alpha)A(\beta). \tag{A.15}$$

This is our promised algebraic relation. Now we can continue and prove the more interesting claim that $B(\beta_1)B(\beta_2)|\omega\rangle$ is in fact an eigenstate to $Z(\alpha) = A(\alpha) + D(\alpha)$:

$$\begin{aligned}
& (A(\alpha)+D(\alpha))B(\beta_1)B(\beta_2)|\omega\rangle \\
= \;& (u(\beta_1-\alpha)B(\beta_1)A(\alpha) + v(\beta_1-\alpha)B(\alpha)A(\beta_1))B(\beta_2)|\omega\rangle \\
+ \;& (u(\alpha-\beta_1)B(\beta_1)D(\alpha) + v(\alpha-\beta_1)B(\alpha)D(\beta_1))B(\beta_2)|\omega\rangle \\
= \;& (u(\beta_1-\alpha)u(\beta_2-\alpha)B(\beta_1)B(\beta_2)A(\alpha)|\omega\rangle \\
+ \;& u(\beta_1-\alpha)v(\beta_2-\alpha)B(\beta_1)B(\alpha)A(\beta_2))|\omega\rangle \\
+ \;& (v(\beta_1-\alpha)u(\beta_1-\beta_2)B(\alpha)B(\beta_2)A(\beta_1)|\omega\rangle \\
+ \;& v(\beta_1-\alpha)v(\beta_2-\beta_1)B(\alpha)B(\beta_1)A(\beta_2))|\omega\rangle \\
+ \;& (u(\alpha-\beta_1)u(\alpha-\beta_2)B(\beta_1)B(\beta_2)D(\alpha)|\omega\rangle \\
+ \;& u(\alpha-\beta_1)v(\alpha-\beta_2)B(\beta_1)B(\alpha)D(\beta_2))|\omega\rangle \\
+ \;& (v(\alpha-\beta_1)u(\beta_2-\beta_1)B(\alpha)B(\beta_2)D(\beta_1)|\omega\rangle \\
+ \;& v(\alpha-\beta_1)v(\beta_1-\beta_2)B(\alpha)B(\beta_1)D(\beta_2))|\omega\rangle \\
= \;& *
\end{aligned} \tag{A.16}$$

Now we use eqn. (A.3) and shuffle around the terms:

$$\begin{aligned}
* &= (u(\beta_1-\alpha)u(\beta_2-\alpha)B(\beta_1)B(\beta_2)A(\alpha)|\omega\rangle \\
&+ u(\alpha-\beta_1)u(\alpha-\beta_2)B(\beta_1)B(\beta_2)D(\alpha))|\omega\rangle \\
&+ (u(\beta_1-\alpha)v(\beta_2-\alpha)+v(\beta_1-\alpha)v(\beta_2-\beta_1))B(\alpha)B(\beta_1)A(\beta_2)|\omega\rangle \\
&+ (u(\alpha-\beta_1)v(\alpha-\beta_2)+v(\alpha-\beta_1)v(\beta_1-\beta_2))B(\alpha)B(\beta_1)D(\beta_2)|\omega\rangle \\
&+ (v(\beta_1-\alpha)u(\beta_2-\beta_1)B(\alpha)B(\beta_2)A(\beta_1)|\omega\rangle \\
&+ v(\alpha-\beta_1)u(\beta_1-\beta_2)B(\alpha)B(\beta_2)D(\beta_1))|\omega\rangle \\
&= **
\end{aligned}$$

By some simple algebraic calculations it is easy to show that

$$u(\beta_1-\alpha)v(\beta_2-\alpha)+v(\beta_1-\alpha)v(\beta_2-\beta_1) = v(\beta_2-\alpha)u(\beta_1-\beta_2) \quad \text{(A.17)}$$

$$u(\alpha-\beta_1)v(\alpha-\beta_2)+v(\alpha-\beta_1)v(\beta_1-\beta_2) = -v(\beta_2-\alpha)u(\beta_2-\beta_1). \quad \text{(A.18)}$$

Finally, by noting that $v(-\alpha) = -v(\alpha)$, we obtain

$$\begin{aligned}
** &= (u(\beta_1-\alpha)u(\beta_2-\alpha)+\Delta(\alpha)u(\alpha-\beta_1)u(\alpha-\beta_2))B(\beta_1)B(\beta_2)|\omega\rangle \\
&+ (v(\beta_1-\alpha)[u(\beta_2-\beta_1)-u(\beta_1-\beta_2)\Delta(\beta_1)]))B(\alpha)B(\beta_2)|\omega\rangle \\
&+ (v(\beta_2-\alpha)[u(\beta_1-\beta_2)-u(\beta_2-\beta_1)\Delta(\beta_2)])B(\alpha)B(\beta_1)|\omega\rangle \\
&\equiv \lambda(\alpha,\beta_1,\beta_2)B(\beta_1)B(\beta_2)|\omega\rangle + \lambda_1(\alpha,\beta_1,\beta_2)B(\alpha)B(\beta_2)|\omega\rangle \\
&+ \lambda_2(\alpha,\beta_1,\beta_2)B(\alpha)B(\beta_1)|\omega\rangle \quad \text{(A.19)}
\end{aligned}$$

If we choose β_1 and β_2 such that λ_1 and λ_2 are equal to zero then $B(\beta_1)B(\beta_2)|\omega\rangle$ is indeed an eigenstate to $Z(\alpha) = A(\alpha) + D(\alpha)$. We thus add the condition

$$\lambda_\gamma(\alpha,\beta_1,\cdots,\beta_M) = 0 \quad \gamma = 1,2 \quad \text{(A.20)}$$

As shown in the main text, sect. (3.4), the condition eqn. (A.20) leads to the famous Bethe Ansatz equations [22].

Appendix B

Mathematical appendix

In this appendix we will introduce some theory about integral equations. We start with a simple case. Given the integral equation

$$f(x) = g(x) + \lambda \int_{-\infty}^{\infty} K(x-y) f(y) dy, \tag{B.1}$$

we can try to solve it by using the Fourier transform

$$\tilde{f}(\omega) = \int_{-\infty}^{\infty} dx f(x) e^{-i\omega x}. \tag{B.2}$$

The Fourier transform of eqn. (B.1) is

$$\tilde{f}(\omega) = \tilde{g}(\omega) + \lambda \tilde{K}(\omega) \tilde{f}(\omega). \tag{B.3}$$

So we have

$$\tilde{f}(\omega) = \frac{\tilde{g}(\omega)}{1 - \lambda \tilde{K}(\omega)}. \tag{B.4}$$

Hence we can solve the integral equation eqn. (B.1) if we can find the inverse fourier transform of eqn. (B.4).

B.1 Pertubation theory

If we have an integral equation of the form

$$f(x) = g(x) + \lambda \int_{a}^{b} K(x,y) f(y) dy \tag{B.5}$$

we can make the approximation $f(x) \approx f(x_0) = g(x)$ to zeroth order. If we now take this crude estimate and put it back into the integral we obtain

$$f_1(x) = g(x) + \lambda \int_a^b K(x,z) f_0(z) dz = g(x) + \lambda \int_a^b K(x,z) g(z) dz. \tag{B.6}$$

This is the first order approximation in λ. If we repeat the procedure we obtain the second order approximation

$$\begin{aligned} f_2(x) &= g(x) + \lambda \int_a^b K(x,z) f_1(z) dz \qquad \text{(B.7)} \\ &= g(x) + \lambda \int_a^b K(x,z_1) g(z_1) dz_1 + \lambda_2 \int_a^b dz_1 \int_a^b dz_2 K(x,z_1) K(z_1,z_2) g(z_2). \end{aligned}$$

Continuing this process we obtain higher-order approximations. If we introduce the functions

$$K_1(x,z) = K(x,z) \qquad \text{(B.8)}$$

$$K_2(x,z) = \int_a^b dz_1 K(x,z_1) K(z_1,z) \qquad \text{(B.9)}$$

$$K_3(x,z) = \int_a^b dz_1 \int_a^b dz_2 K(x,z_1) K(z_1,z_2) K(z_2,z) \qquad \text{(B.10)}$$

and so on, obeying the reccurence relation

$$K_n(x,z) = \int_a^b K(x,z_1) K_{n-1}(z_1,z) dz_1, \qquad \text{(B.11)}$$

we can write the nth-order approximation as

$$f_n(x) = g(x) + \sum_{m=1}^{n} \lambda^n \int_a^b K_m(x,z) g(z) dz. \qquad \text{(B.12)}$$

B.2 Wiener-Hopf method

A more difficult integral equation is that which is of Wiener-Hopf type. It has the form

$$p(x) = p^{(0)}(x) + \int_0^\infty K(x-x') p(x') dx', \qquad \text{(B.13)}$$

with the integration confined to the half-line $[0,\infty)$. We start by taking the Fourier transform of eqn. (B.13):

$$(1 - K(\omega)) p^+(\omega) + p^-(\omega) = p^{(0)}(\omega), \qquad \text{(B.14)}$$

here

$$p^\pm = \int dz \theta_H(\pm z) p(z) e^{i\omega z} \qquad \text{(B.15)}$$

with z a complex variable taking values in the complex plane. This gives us a decomposition of $p(\omega)$ into two parts which are analytic in the upper and lower half plane, respectively. The key to the solution is now to decompose the kernel into factors $G^\pm$ that are analytical in the upper and lower complex ω-plane, respectively:

$$1 - R(\omega) = (G^+(\omega) G^-(\omega))^{-1}, \qquad \lim_{\omega \to \infty} G^\pm(\omega) = 1. \qquad \text{(B.16)}$$

If we use this factorization eqn. (B.14) can be rewritten as

$$(G^+(\omega))^{-1}p^+(\omega) + G^-(\omega)p^-(\omega) = Q^+(\omega) + Q^-(\omega). \tag{B.17}$$

Here $Q^{\pm}(\omega)$ are analytic in the upper and lower half planes respectively and given by

$$Q^+(\omega) + Q^-(\omega) = G^-(\omega)p^{(0)}(\omega). \tag{B.18}$$

If we now use the analytic properties of the functions $G^{\pm}$ and $Q^{\pm}$ we can obtain a solution of eqn. (B.17) on the form

$$p^+(\omega) = G^+(\omega)Q^+(\omega) \tag{B.19}$$

$$p^-(\omega) = \frac{Q^-(\omega)}{G^-(\omega)}. \tag{B.20}$$

For later use we also define the following indetities:

$$\int_0^\infty p(x)dx = p^+(\omega = 0) \tag{B.21}$$

$$\int_0^\infty e^{-\frac{\pi x}{2}}p(x)dx = p^+(-\frac{i\pi}{2}). \tag{B.22}$$

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