Derivation of the pCUT U
Application to topological order

Bachelor's Thesis in Physics

Presented by

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Abstract

In this work the method of perturbative continuous unitary transformation is derived and altered in order to specifically calculate the unitary transformation leading to the effective Hamiltonian. The result is a system of recursive differential equations for the coefficient functions of the effective Hamiltonian and the effective unitary transformation. It then can be solved using a computer program, that is optimized by using certain properties of the coefficient functions. The usefulness of these calculations is demonstrated by applying it to the toric code model in a magnetic field, which is a system often considered to study the robustness of topological order with respect to external influences. The effective Hamiltonian is used to calculate the ground-state energy of the toric code and the evolution of an excited state. The effective unitary transformation is used to show that the topologically ordered ground states of the toric code are stable with respect to a low magnetic field.

Contents

1 Introduction

Systems with topological order have highly entangled ground states that depend on the topology of the underlying lattice. They have a degenerate ground-state manifold that is stable against local perturbations, as was proven by Bravyi, Hastings and Michalakis ([1], [2]). A prominent example for a system with topological order is the toric code. It is an exactly solvable model, introduced by Kitaev ([3]). One approach to study the robustness of topologically-ordered ground states of this system is by applying external perturbation. One possible method applicable here is the method of perturbative continuous unitary transformation (pCUT) ([4], [5], [6]). This formalism allows to calculate a quasi-particle-conserving effective Hamiltonian, in order to investigate the low-energy physics of a system. Dusuel, Schmidt, Thomale and Vidal used pCUT to show that the ground states of the toric code are stable against different configurations of magnetic fields ([7], [8]). Furthermore, it is possible to alter the pCUT formalism and to calculate the effective unitary transformation directly, as Halász and Hamma did ([9]).

In the first part of this thesis, we will cover the pCUT formalism and the effective unitary transformation. In chapter 2, we will derive the unaltered pCUT formalism. The result will be a system of recursive differential equations that can be solved using a computer program. In order to implement such a program efficiently, we will find simplifications and reduce the number of necessary calculations. We will calculate the results by hand up to second order to understand the nature of these calculations. In chapter 3, we will derive the formalism that allows to calculate the unitary transformation directly. The result will be a system of recursive differential equations that also depends on the results of chapter 2. These equations can also be solved recursively by the same computer program after extending it. We will again find simplifications to reduce the number of necessary calculations and calculate the results up to second order. The next part of this thesis will cover the toric code. In chapter 4, we will introduce the toric code and examine its ground-state manifold and the first excited states in detail. In chapter 5, we will perturb this system with a low magnetic field and calculate the effective Hamiltonian up to second order using the results from chapter 2. We will use this in order to calculate the ground-state energy and the evolution of the first excited state. Then we will calculate the effective unitary transformation up to second order using the results from chapter 3. In the

end we will use this transformation in order to calculate that the ground states of the toric code are stable against the perturbation of a low magnetic field.

2 pCUT formalism

Wegner introduced in [4] the formalism of continuous unitary transformations (CUTs). The goal is to perform a unitary transformation leading to an effective Hamiltonian in a continuous way. The transformation is determined by the choice of its infinitesimal generator. Independently, Mielke and Knetter and Uhrig found a generator suitable for a band-diagonal Hamiltonian in [5] and [6]. This transformation can be approached perturbatively (pCUT) if the unperturbed Hamiltonian has an equidistant spectrum that is bounded from below and if the perturbing Hamiltonian changes the number of quasi-particles in a limited way. Then the generated effective Hamiltonian is block-diagonal and therefore quasi-particle conserving. A quasi-particle conserving Hamiltonian is suited for the analysis of low-energy physics.

2.1 CUT formalism

Wegner introduced the continuous flow parameter ℓ, running from 0 to ∞ and the Hamiltonian $H(\ell)$ that transforms unitarily from the original Hamiltonian H to the effective one H_{eff}. This transformation is realized using a continuous unitary operator $U(\ell)$ and defining the transforming Hamiltonian as $H(\ell) := U^\dagger(\ell) H U(\ell)$. Every continuous unitary operator has an antihermitian infinitesimal generator $\eta(\ell)$ such that

$$\frac{\mathrm{d}U(\ell)}{\mathrm{d}\ell} = -U(\ell)\eta(\ell). \tag{2.1}$$

The calculation

$$0 = \frac{\mathrm{d}\mathbb{1}}{\mathrm{d}\ell} = \frac{\mathrm{d}(U^\dagger(\ell)U(\ell))}{\mathrm{d}\ell} = \frac{\mathrm{d}U^\dagger(\ell)}{\mathrm{d}\ell}U(\ell) + U^\dagger(\ell)\frac{\mathrm{d}U(\ell)}{\ell}.$$

can be used to check that the generator

$$\eta(\ell) = -U^\dagger(\ell)\frac{\mathrm{d}U(\ell)}{\mathrm{d}\ell} = \frac{\mathrm{d}U^\dagger(\ell)}{\mathrm{d}\ell}U(\ell) = -\eta^\dagger(\ell)$$

is in fact antihermitian.

The condition $H(\ell) = U^\dagger(\ell) H U(\ell)$ implies

$$\begin{aligned}
\frac{\mathrm{d}H(\ell)}{\mathrm{d}\ell} &= \frac{\mathrm{d}U^\dagger(\ell)}{\mathrm{d}\ell} H U(\ell) + U^\dagger(\ell) H \frac{\mathrm{d}U(\ell)}{\mathrm{d}\ell} \\
&= \frac{\mathrm{d}U^\dagger(\ell)}{\mathrm{d}\ell} U(\ell) U^\dagger(\ell) H U(\ell) + U^\dagger(\ell) H U(\ell) U^\dagger(\ell) \frac{\mathrm{d}U(\ell)}{\mathrm{d}\ell} \\
&= \frac{\mathrm{d}U^\dagger(\ell)}{\mathrm{d}\ell} U(\ell) H(\ell) + H(\ell) U^\dagger(\ell) \frac{\mathrm{d}U(\ell)}{\mathrm{d}\ell} \\
&= -U^\dagger(\ell) \frac{\mathrm{d}U(\ell)}{\mathrm{d}\ell} H(\ell) + H(\ell) U^\dagger(\ell) \frac{\mathrm{d}U(\ell)}{\mathrm{d}\ell} = \left[-U^\dagger(\ell) \frac{\mathrm{d}U(\ell)}{\mathrm{d}\ell}, H(\ell) \right].
\end{aligned}$$

Using the generator, the Hamiltonian transforms according to the flow equation

$$\frac{\mathrm{d}H(\ell)}{\mathrm{d}\ell} = [\eta(\ell), H(\ell)]. \tag{2.2}$$

The choice of the generator influences the form of the effective Hamiltonian. Knetter and Uhrig developed a generator that generates a quasi-particle conserving Hamiltonian. In second quantization, the generator can be written as

$$\eta(\ell) = \sum_{i,j} \mathrm{sgn}(i-j) H^i_j(\ell), \tag{2.3}$$

where $H^i_j(\ell)$ is the block of the Hamiltonian that creates i and annihilates j quasi-particles.

2.2 Ansatz

In general, it can be very complicated to find a solution to the flow equation (2.2). For some systems, it is possible to use a perturbative ansatz, denoted by pCUT formalism. The pCUT formalism can be applied if the unperturbed Hamiltonian H_0 has an equidistant spectrum bounded from below and if the perturbing Hamiltonian increments or decrements the energy of an eigenstate of H_0 by at most N energy quanta, where N is a natural number. More specific, if the Hamiltonian is of the form

$$H = H_0 + \lambda \sum_{n=-N}^{N} T_n, \tag{2.4}$$

with $[H_0, T_n] = n T_n$. The operators T_n increment the energy of an eigenstate of H_0 by n. It holds that $T_n^\dagger = T_{-n}$, because the Hamiltonian has to be self-adjoint. The flow equation (2.2) and the definition of the generator (2.3) motivate the ansatz

$$H(\ell) = H_0 + \sum_{k=1}^{\infty} \lambda^k \sum_{|\underline{m}|=k} F(\ell; \underline{m}) T(\underline{m}), \tag{2.5}$$

where k denotes the order, $\underline{m}$ are tuples defined as $\underline{m} := (m_1, \ldots, m_k)$ with values $m_i \in \{-N, \ldots, N\}$, $F(\ell; \underline{m})$ are real-valued coefficient functions and $T(\underline{m})$ is defined as $T(\underline{m}) := T_{m_1} \cdot \ldots \cdot T_{m_k}$. The equation

$$\begin{aligned}
[H_0, T(\underline{m})] &= [H_0, T_{m_1} T_{m_2} T_{m_3} \cdot \ldots \cdot T_{m_k}] \\
&= [H_0, T_{m_1}] T_{m_2} T_{m_3} \cdot \ldots \cdot T_{m_k} + T_{m_1} [H_0, T_{m_2} T_{m_3} \cdot \ldots \cdot T_{m_k}] \\
&= m_1 T(\underline{m}) + T_{m_1} [H_0, T_{m_2}] T_{m_3} \cdot \ldots \cdot T_{m_k} + T_{m_1} T_{m_2} [H_0, T_{m_3}, \cdot \ldots \cdot T_{m_k}] \\
&= m_1 T(\underline{m}) + m_2 T(\underline{m}) + \ldots + m_k T(\underline{m}) \\
&= (m_1 + \ldots + m_k) T(\underline{m}) =: M(\underline{m}) T(\underline{m}).
\end{aligned}$$

suggests that equation (2.5) is a generalization of equation (2.4). The generator from equation (2.3) becomes

$$\eta(\ell) = \sum_{k=1}^{\infty} \lambda^k \sum_{|\underline{m}|=k} \operatorname{sgn}(M(\underline{m})) F(\ell; \underline{m}) T(\underline{m}). \tag{2.6}$$

The unperturbed Hamiltonian H_0 is not present in the definition of the generator, because it does not change the number of quasi-particles.

The effective Hamiltonian H_{eff} is given by

$$H_{\text{eff}} = H(\infty) = H_0 + \sum_{k=1}^{\infty} \lambda^k \sum_{|\underline{m}|=k} F(\infty; \underline{m}) T(\underline{m}).$$

We will see that $F(\infty; \underline{m}) = 0$ for $M(\underline{m}) \neq 0$, which is why the resulting effective Hamiltonian is quasi-particle conserving. Please note that the coefficients $F(\infty, \underline{m})$ are model-independent. The information about the model is contained in the unperturbed Hamiltonian H_0 and in the specific definition of the operators T_n. We can therefore calculate the coefficient functions once and apply our results to all systems with the same type of perturbation in the sense that the maximally incremented or decremented energy is the same.

2.3 Differential equations

The flow equation (2.2) together with the ansatz from equation (2.5) can be used to calculate the coefficient functions F. Inserting the ansatz into the left-hand side of the flow equation yields

$$\frac{\mathrm{d}H(\ell)}{\mathrm{d}\ell} = \sum_{k=1}^{\infty} \lambda^k \sum_{|\underline{m}|=k} \frac{\mathrm{d}F(\ell; \underline{m})}{\mathrm{d}\ell} T(\underline{m}).$$

Using $[H_0, T(\underline{m})] = M(\underline{m})T(\underline{m})$ and inserting the ansatz and the generator into the right-hand side of the generator yields

$$\begin{aligned}
[\eta(\ell), H(\ell)] = &\sum_{k_\eta=1}^{\infty} \lambda^{k_\eta} \sum_{|\underline{m}_\eta|=k_\eta} \operatorname{sgn}(M(\underline{m}_\eta))F(\ell;\underline{m}_\eta)[T(\underline{m}_\eta), H_0] \\
&+ \sum_{k_\eta,k_H=1}^{\infty} \lambda^{k_\eta+k_H} \sum_{|\underline{m}_\eta|=k_\eta} \sum_{|\underline{m}_H|=k_H} \operatorname{sgn}(M(\underline{m}_\eta))F(\ell;\underline{m}_\eta)F(\ell;\underline{m}_H) \\
&\qquad \times [T(\underline{m}_\eta), T(\underline{m}_H)] \\
= &- \sum_{k=1}^{\infty} \lambda^{k} \sum_{|\underline{m}|=k} |(M(\underline{m})|F(\ell;\underline{m})T(\underline{m}) \\
&+ \sum_{k=2}^{\infty} \lambda^{k} \sum_{|\underline{m}|=k} \sum_{(\underline{m}_1,\underline{m}_2)=\underline{m}} [\operatorname{sgn}(M(\underline{m}_1)) - \operatorname{sgn}(M(\underline{m}_2))] \\
&\qquad \times F(\ell;\underline{m}_1)F(\ell;\underline{m}_2)T(\underline{m}),
\end{aligned}$$

where $(\underline{m}_1, \underline{m}_2) = \underline{m}$ denotes all non-trivial breakups of $\underline{m}$. The whole flow equation can be used to obtain the following system of differential equations for the coefficient functions

$$\begin{aligned}
\frac{\mathrm{d}F(\ell;\underline{m})}{\mathrm{d}\ell} = &- |M(\underline{m})|F(\ell;\underline{m}) \\
&+ \sum_{(\underline{m}_1,\underline{m}_2)=\underline{m}} [\operatorname{sgn}(M(\underline{m}_1)) - \operatorname{sgn}(M(\underline{m}_2))]F(\ell;\underline{m}_1)F(\ell;\underline{m}_2). \qquad (2.7)
\end{aligned}$$

The condition $H(0) = H$ implies the starting conditions $F(0;\underline{m}) = \delta_{|\underline{m}|,1}$.

For $\underline{m} = (m_1)$, equation (2.7) simplifies to

$$\frac{\mathrm{d}F(\ell;(m_1))}{\mathrm{d}\ell} = -|m_1|F(\ell;(m_1)),$$

because there are no non-trivial breakups of (m_1). Together with the starting conditions, the result is $F(\ell;(m_1)) = e^{-|m_1|\ell}$.

The system of coupled differential equations (2.7) is solved by functions of the form $F(\ell;\underline{m}) = e^{-|M(\underline{m})|\ell} f(\ell;\underline{m})$. The new coefficient functions f can be calculated by the system of recursive differential equations

$$\begin{aligned}
\frac{\mathrm{d}f(\ell;\underline{m})}{\mathrm{d}\ell} = &\sum_{(\underline{m}_1,\underline{m}_2)=\underline{m}} e^{(|(M(\underline{m})|-|M(\underline{m}_1)|-|M(\underline{m}_2)|)\ell} \\
&\qquad \times [\operatorname{sgn}(M(\underline{m}_1)) - \operatorname{sgn}(M(\underline{m}_2))]f(\ell;\underline{m}_1)f(\ell;\underline{m}_2). \qquad (2.8)
\end{aligned}$$

The starting conditions of the new functions are $f(0;\underline{m}) = \delta_{|\underline{m}|,1}$ as before and $f(\ell;(m_1)) = 1$. Because of the factor $e^{-|M(\underline{m})|\ell}$ in the relation between $F(\ell;\underline{m})$ and

$f(\ell;\underline{m})$ the coefficients $F(\infty;\underline{m})$ will vanish for $M(\underline{m}) \neq 0$. This can only hold if the function $f(\ell;\underline{m})$ does not contain exponentially growing factors, but we will see in section 2.5 that it does not.

2.4 Symmetry relations

The coefficient functions obey certain symmetry relations, namely

1. $F(\ell;-(m_k,\dots,m_1)) = F(\ell;(m_1,\dots,m_k))$.

2. $F(\ell;-\underline{m}) = (-1)^{|\underline{m}|-1}F(\ell;\underline{m})$.

The functions f obey these symmetry relations too. We will prove them for the functions F by proving them for the functions f via induction on $|\underline{m}|$. We already saw that $f(\ell;-(m_1)) = 1 = f(\ell;(m_1))$, which is the base case for the first two symmetry relations. Our induction hypothesis is that the symmetry relations hold for all functions $f(\ell;\underline{m})$ with $|\underline{m}| < k$. Now let $\underline{m}$ be arbitrary with $|\underline{m}| = k$. We will carry out the induction step using equation (2.8) and the condition $f(0;\underline{m}) = \delta_{|\underline{m}|,1}$.

1. The breakup $((m_1,\dots,m_i),(m_{i+1},\dots m_k))$ of $(m_1,\dots,m_k)$ and the breakup $((-m_k,\dots,-m_{i+1}),(-m_i,\dots,m_1))$ of $-(m_k,\dots,m_1)$ generate the same term in equation (2.8). The exponential factor is the same for both breakups because of the absolute values. The factor $f(\ell;\underline{m}_1)f(\ell;\underline{m}_2)$ is also the same because of the induction hypothesis. The factor $\operatorname{sgn}(M(\underline{m}_1)) - \operatorname{sgn}(M(\underline{m}_2))$ is more difficult. The minus signs in front of the second breakup generate a total minus sign in contrast to the first breakup, which is compensated by a second minus sign emerging from the reversed order of the values in the second breakup. In total, the whole term is equal for both breakups. This holds for every possible breakup. Therefore, equation (2.8) is equal for $f(\ell;(m_1,\dots,m_k))$ and $f(\ell;-(m_k,\dots,m_1))$. The starting condition for the functions depends only on k and not on the order or sign of the values, which is why the two functions are the same.

2. We do not have to consider the exponential factor for the second property, because it does not depend on the sign in front of $\underline{m}$. Using the induction hypothesis, it holds that

$$\begin{aligned}
&[\operatorname{sgn}(M(-\underline{m}_1)) - \operatorname{sgn}(M(-\underline{m}_2))]f(\ell;-\underline{m}_1)f(\ell;-\underline{m}_2)\\
=&-[\operatorname{sgn}(M(\underline{m}_1)) - \operatorname{sgn}(M(\underline{m}_2))](-1)^{|\underline{m}_1|-1}f(\ell;\underline{m}_1)(-1)^{|\underline{m}_2|-1}f(\ell;\underline{m}_2)\\
=&(-1)^{|\underline{m}|-1}[\operatorname{sgn}(M(\underline{m}_1)) - \operatorname{sgn}(M(\underline{m}_2))]f(\ell;\underline{m}_1)f(\ell;\underline{m}_2).
\end{aligned}$$

That is why equation (2.8) is the same for $f(\ell; -\underline{m})$ and $(-1)^{|\underline{m}|-1} f(\ell; \underline{m})$. The starting conditions are also the same for both functions. That is because for $|\underline{m}| = 1$, it holds that $(-1)^{|\underline{m}|-1} = 1$ and for $|\underline{m}| > 1$, the functions have to vanish anyway. Therefore the two functions $f(\ell; -\underline{m})$ and $(-1)^{|\underline{m}|-1} f(\ell; \underline{m})$ are equal.

The functions F and the functions f differ by a factor of $e^{-|M(\underline{m})|\ell}$. This factor is neither depending on the sign in front of $\underline{m}$ nor on the order of the elements of $\underline{m}$. Therefore the two symmetry relations also hold for the functions F. Please note that the first one is equivalent to the fact that the Hamiltonian has to be self-adjoint, which can be seen immediately from the fact that $T_n^\dagger = T_{-n}$ and from the definition of $T(\underline{m})$.

2.5 Properties

The coefficient functions $F(\ell; \underline{m})$ vanish for $|M(\underline{m})| > N$. the same holds for the functions f for which we will prove this property first via induction on $|\underline{m}|$. The base case is trivially fulfilled, because there are no (m_1) with $|M((m_1))| = |m_1| > N$. Our induction hypothesis is that all functions $f(\ell; \underline{m})$ with $|\underline{m}| < k$ vanish for $|M(\underline{m})| > N$. Now let $\underline{m}$ be arbitrary with $|\underline{m}| = k > 1$ and $|M(\underline{m})| > N$. We will carry out the induction step using equation (2.8) and the condition $f(0; \underline{m}) = \delta_{|\underline{m}|,1}$. Let (m_1, m_2) be an arbitrary non-trivial breakup of $\underline{m}$. Because of our induction hypothesis, the corresponding term in equation (2.8) is only non-vanishing if $|M(\underline{m}_1)| \leq N$ and $|M(\underline{m}_2)| \leq N$. Because of $N < M(\underline{m}) = M(\underline{m}_1) + M(\underline{m}_2)$ both, $M(m_1)$ and $M(m_2)$, have to be positive and the term vanishes nonetheless. Analogously, every term vanishes if $M(\underline{m}) < -N$. Together with the starting condition $f(0; \underline{m}) = 0$, this leads for $|M(\underline{m})| > N$ to $f(\ell; \underline{m}) = 0$. If one of the functions $f(\ell; \underline{m})$ vanishes, the corresponding coefficient function $F(\ell; \underline{m})$ does too. That is why the coefficient functions $F(\ell; \underline{m})$ vanish for $|M(\underline{m})| > N$.

The functions f are of the form

$$f(\ell; \underline{m}) = \sum_{\mu \geq 0} P_\mu(\ell; \underline{m}) e^{-\mu\ell} \tag{2.9}$$

with non-negative integers μ and polynomials $P_\mu(\ell; \underline{m})$ with rational coefficients. The upper bound of this sum is not important for our case, but it is obvious that it is finite for every function. We can prove equation (2.9) via induction on $|\underline{m}|$ using equation (2.8) and the starting conditions $f(0; \underline{m}) = \delta_{|\underline{m}|,1}$. We have already seen in section 2.3 that $f(\ell; (m_1)) = 1$ which is of the form described in (2.9) with $P_0(\ell; (m_1)) = 1$. This is our basecase. Our induction hypothesis is that all functions $f(\ell; \underline{m})$ with $|\underline{m}| < k$

can be written as in equation (2.9). Let $\underline{m}$ be such that $|\underline{m}| = k > 1$. According to equation (2.8), $f(\ell; \underline{m})$ is given by

$$f(\ell;\underline{m}) = \sum_{(\underline{m}_1,\underline{m}_2)=\underline{m}} \int e^{(|(M(\underline{m})|-|M(\underline{m}_1)|-|M(\underline{m}_2)|)\ell} [\operatorname{sgn}(M(\underline{m}_1)) - \operatorname{sgn}(M(\underline{m}_2))] \times f(\ell;\underline{m}_1) f(\ell;\underline{m}_2) \mathrm{d}\ell. \tag{2.10}$$

Because the term $|M(\underline{m})|-|M(\underline{m}_1)|-|M(\underline{m}_2)|$ is always non-negative, the integrand is again of the form (2.9) and therefore also the function

$$f(\ell;\underline{m}) = \sum_{\mu \geq 0} P_\mu(\ell;\underline{m}) e^{-\mu\ell} + c.$$

The starting condition implies that $c = -\sum_{\mu\geq 0} P_\mu(0;\underline{m})$. In total, the function f is of the form

$$f(\ell;\underline{m}) = P_0(\ell;\underline{m}) - \sum_{\mu\geq 0} P_\mu(0;\underline{m}) + \sum_{\mu\geq 1} P_\mu(\ell;\underline{m}) e^{-\mu\ell},$$

which is again of the form stated in equation (2.9). Here we also see that the functions f do not contain exponentially growing factors and therefore that the coefficients $F(\infty;\underline{m})$ vanish for $M(\underline{m}) \neq 0$.

The coefficients $F(\infty;\underline{m})$ have to be finite for the transformation to converge. For that we have to prove that the polynomials $P_0(\ell;\underline{m})$ are constant if $M(\underline{m}) = 0$. This is the case, because $P_0(\ell;\underline{m})$ is equal to the constant of integration from equation (2.10). If $\underline{m}$ is such that $M(\underline{m}) = 0$ and if $(\underline{m}_1, \underline{m}_2)$ is an arbitrary non-trivial breakup of $\underline{m}$, then it holds that $M(\underline{m}_1) + M(\underline{m}_2) = M(\underline{m}) = 0$ and therefore that $M(\underline{m}_2) = -M(\underline{m}_2)$. Using that, the exponential term becomes $e^{-2|M(\underline{m}_1)|\ell}$ and the sign-factor becomes $2\operatorname{sgn}(M(\underline{m}_1))$. If the breakup is such that $M(\underline{m}_1) = 0$, then the whole term vanishes due to the sign-factor. If $M(\underline{m}_1) \neq 0$, then the term is exponentially decreasing and does not contribute to $P_0(\ell;\underline{m})$. Therefore the only term left for $P_0(\ell;\underline{m})$ is the constant of integration.

2.6 Implementation

It is easier to calculate the functions f first and then the coefficient functions F from them. Because these functions are of the shape stated in equation (2.9), they can be calculated using an algorithm from Knetter that is described in more detail in [10] and [6].

Because the system of differential equations (2.8) is recursive, one can implement the program order by order using a loop or recursion. Knetter's algorithm uses the

former. For each order k it is possible to invertibly map all possible tuples $\underline{m}$ onto the integer numbers between 0 and $\widetilde{N}^k - 1$, where $\widetilde{N}$ is the number of non-vanishing T_n operators. This is accomplished by converting the tuples into representations of natural numbers using the base-$\widetilde{N}$ numeral system. For that, we first map each tuple $\underline{m}$ onto the tuple $\underline{a}$ by defining $a_i := a(m_i)$, where a is an arbitrary bijection from $\{-N, \dots, N\}$ to $\{0, \dots, \widetilde{N} - 1\}$. Then we calculate the desired integers via $\sum_{i=0}^{\widetilde{N}} a_i \widetilde{N}^i$, which is the conversion of the base-$\widetilde{N}$ numeral system to the natural numbers. These numbers can be used for the next loop to calculate the functions $f(\ell; \underline{m})$ of the same order one after another. Since the functions of the same order do not depend on one another, this procedure is parallelizable.

Because of the shape of the functions f stated in equation (2.9), they can be stored as a list of quasipolynomials. Each quasipolynomial is represented by four integers – the nominator and the denominator of the prefactor, the power of ℓ and the integer μ in the exponential. The data types for the exponential integers and the powers need not store big integers, but the prefactors can become very large. Using this representation of quasipolynomials, operations like integration or addition can be implemented rather easily. Two quasipolynomials are multiplied by multiplying the nominators and the denominators and by adding the powers and the exponential integers. The calculation

$$\int_0^\ell \frac{p}{q} \ell'^i e^{-\mu \ell'} \mathrm{d}\ell' = \begin{cases} \dfrac{p}{q(1+i)} \ell^{i+1} & \text{for } \mu = 0 \\ \dfrac{pi!}{q\mu} \left(\dfrac{1}{\mu^i} - e^{-\mu\ell} \displaystyle\sum_{j=0}^{i} \frac{\ell^j}{j! \mu^{i-j}} \right) & \text{for } \mu > 0 \end{cases}$$

depicts how the stored integers have to be modified when integrating. The second term in this calculation contains more than one summand, which means that more quasipolynomials have to be added to the list.

When a function $f(\ell; \underline{m})$ is calculated, the corresponding coefficient function is given by $F(\ell; \underline{m}) = e^{-|M(\underline{m})|\ell} f(\ell; \underline{m})$. For the effective Hamiltonian, we are only interested in the coefficients $F(\infty; \underline{m})$. Only coefficients with $M(\underline{m}) = 0$ will not vanish, so we only need to write them into the file containing the results. For $M(\underline{m}) = 0$ it holds that $F(\ell; \underline{m}) = f(\ell; \underline{m})$, so the coefficients are easy to extract from the quasipolynomials, as they are given by the prefactor of the quasimonomial with $\mu = 0$.

The overall required RAM storage can be minimized using the symmetry relations. Only about one quarter of the functions have to be saved, because the remaining functions can be derived before inserting them into equation (2.8). Time can be saved when functions $f(\ell; \underline{m})$ with $|M(\underline{m})| > N$ are omitted because they vanish

anyway, as we proved in section 2.5. When calculating the function of the maximal desired order, it suffices to calculate those with $M(\underline{m}) = 0$. These results can be written onto the file right away, because they are not needed in order to calculate more functions.

2.7 Results up to second order

Calculating the coefficient functions F for arbitrary N can be done by hand rather quickly up to second order. The first order is particularly simple, as we already saw in section 2.3. The coefficient functions are given by $F(\ell;(m_1)) = e^{-|m_1|\ell}$ and therefore the first order of the Hamiltonian is given by

$$\sum_{|\underline{m}|=1} F(\ell;\underline{m})T(\underline{m}) = T_0 + \sum_{n=1}^{N} e^{-n\ell}(T_n + T_{-n}).$$

Therefore the effective Hamiltonian up to first order is given by $H_{\text{eff}}^{(1)} = H_0 + \lambda T_0$.

The second order requires more calculation and case differentiation. Because of the sign-factor in equation (2.8), functions $F(\ell;(m_1,m_2))$ with $\operatorname{sgn}(m_1) = \operatorname{sgn}(m_2)$ have to vanish. Let us consider tuples of the form $(n,0)$ with $n > 0$. Then it holds that the exponential in equation (2.8) vanishes, because $|n+0| - |n| - 0 = 0$. Therefore the function $f(\ell;(n,0))$ is given by

$$f(\ell;(n,0)) = \int_0^\ell \mathrm{d}\ell' = 2\ell$$

and it holds that

$$F(\ell;(n,0)) = \ell e^{-n\ell}.$$

Using the symmetry relations from section 2.4, we also derive the functions

$$\begin{aligned} F(\ell;(-n,0)) &= -\ell e^{-n\ell} \\ F(\ell;(0,n)) &= -\ell e^{-n\ell} \\ F(\ell;(0,-n)) &= \ell e^{-n\ell} \end{aligned}$$

without specifically calculating them. We have not regarded tuples like $(n,-m)$ with $n,m > 0$ yet. The corresponding functions f are given by

$$f(\ell;(n,-m)) = \int_0^\ell 2e^{(|n-m|-n-m)\ell'}\mathrm{d}\ell' = \frac{2}{|n-m|-n-m}\left(e^{(|n-m|-n-m)\ell} - 1\right).$$

Together with the symmetry relations, it holds that

$$F(\ell;(n,-m)) = \frac{2}{|n-m|-n-m}\left(e^{-(n+m)\ell} - e^{-|n-m|\ell}\right)$$
$$F(\ell;(-m,n)) = -\frac{2}{|n-m|-n-m}\left(e^{-(n+m)\ell} - e^{-|n-m|\ell}\right).$$

Therefore the second order of the Hamiltonian is given by

$$\sum_{|\underline{m}|=2} F(\ell;\underline{m})T(\underline{m}) = \sum_{n=1}^{N} \ell e^{-n\ell}([T_n,T_0]+[T_0,T_{-n}]) + \sum_{n,m=1}^{N} \frac{2}{|n-m|-n-m}\left(e^{-(n+m)\ell} - e^{-|n-m|\ell}\right)[T_n,T_{-m}]$$

and the effective Hamiltonian up to second order by

$$H_{\text{eff}}^{(2)} = H_0 + \lambda T_0 + \lambda^2 \sum_{n=1}^{N} \frac{1}{n}[T_n,T_{-n}]. \tag{2.11}$$

The commutator in the second order ensures that the action of the Hamiltonian is local, because all processes where one particle is annihilated at one position and one is created at a totally different position are compensated by all processes where one particle is created at one position and one is annihilated at a totally different position.

3 Derivation of the pCUT U

It is possible to calculate the transformation of observables in a way similar to the transformation of the Hamiltonian in equation (2.2). If more observables are required, it is often simpler and faster to calculate the unitary transformation directly and to apply it to the observables afterwards.

3.1 Ansatz and differential equations

The unitary transformation $U(\ell)$ can be calculated via the flow equation (2.1). This equation and the definition of the generator in equation (2.6) justify the ansatz

$$U(\ell) = \mathbb{1} + \sum_{k=1}^{\infty} \lambda^k \sum_{|\underline{m}|=k} G(\ell;\underline{m}) T(\underline{m}),$$

with unknown real-valued coefficient functions $G(\ell;\underline{m})$. Using this ansatz, the left-hand side of the flow equation (2.1) becomes

$$\frac{\mathrm{d}U(\ell)}{\mathrm{d}\ell} = \sum_{k=1}^{\infty} \lambda^k \sum_{|\underline{m}|=k} \frac{\mathrm{d}G(\ell;\underline{m})}{\mathrm{d}\ell} T(\underline{m})$$

and the right-hand side

$$\begin{aligned}
-U(\ell)\eta(\ell) = &- \sum_{k_\eta=1}^{\infty} \lambda^{k_\eta} \sum_{|\underline{m}_\eta|=k_\eta} \operatorname{sgn}(M(\underline{m}_\eta)) F(\ell;\underline{m}_\eta) T(\underline{m}_\eta) \\
&- \sum_{k_U,k_\eta=1}^{\infty} \lambda^{k_U+k_\eta} \sum_{|\underline{m}_U|=k_U} \sum_{|\underline{m}_\eta|=k_\eta} \operatorname{sgn}(M(\underline{m}_\eta)) G(\ell;\underline{m}_U) F(\ell;\underline{m}_\eta) \\
&\qquad \times T(\underline{m}_U) T(\underline{m}_\eta) \\
= &- \sum_{k=1}^{\infty} \lambda^k \sum_{|\underline{m}|=k} \operatorname{sgn}(M(\underline{m})) F(\ell;\underline{m}) T(\underline{m}) \\
&- \sum_{k=2}^{\infty} \lambda^k \sum_{|\underline{m}|=k} \sum_{(\underline{m}_1,\underline{m}_2)=\underline{m}} \operatorname{sgn}(M(m_2)) G(\ell;\underline{m}_1) F(\ell;\underline{m}_2) T(\underline{m}).
\end{aligned}$$

Hence, equation (2.1) yields the system of recursive differential equations for the coefficient functions G

$$\frac{\mathrm{d}G(\ell;\underline{m})}{\mathrm{d}\ell} = -\operatorname{sgn}(M(\underline{m}))F(\ell;\underline{m}) - \sum_{(\underline{m}_1,\underline{m}_2)=\underline{m}} \operatorname{sgn}(M(\underline{m}_2))G(\ell;\underline{m}_1)F(\ell;\underline{m}_2), \tag{3.1}$$

which can be solved if the coefficient functions F up to order $|\underline{m}|$ are known. The condition $H(0) = H$ implies the condition $U(0) = \mathbb{1}$, which in turn implies the starting conditions $G(0;\underline{m}) = 0$. For $\underline{m} = (m_1)$, equation (3.1) simplifies to

$$\frac{\mathrm{d}G(\ell;(m_1))}{\mathrm{d}\ell} = -\operatorname{sgn}(m_1)F(\ell;(m_1)) = -\operatorname{sgn}(m_1)e^{-|m_1|\ell},$$

because there are no non-trivial breakups of (m_1). The final result is

$$G(\ell;(m_1)) = \begin{cases} 0 & \text{for } m_1 = 0, \\ \dfrac{1}{m_1}\left(e^{-|m_1|\ell} - 1\right) & \text{for } m_1 \neq 0, \end{cases}$$

because of the starting conditions.

3.2 Symmetry relation and properties

The coefficient functions G obey the symmetry relation $G(\ell;-\underline{m}) = (-1)^{|\underline{m}|}G(\ell;\underline{m})$, which can be proven via induction on $|\underline{m}|$ using the second symmetry relation of the coefficient functions F and equation (3.1). We already saw that the base case holds, namely that $G(\ell;-(0)) = 0 = G(\ell;(0))$ and that

$$G(\ell;-(m_1)) = \frac{1}{-m_1}\left(e^{-|-m_1|\ell} - 1\right) = -\frac{1}{m_1}\left(e^{-|m_1|\ell} - 1\right) = -G(\ell;(m_1))$$

for $m_1 \neq 0$. Our induction hypothesis is that the symmetry relation holds for all functions $G(\ell;\underline{m})$ with $|\underline{m}| < k$. Now let $\underline{m}$ be arbitrary with $|\underline{m}| = k$. We will carry out the induction step using equation (3.1) and the starting condition $G(0;\underline{m}) = 0$. Let us have a look at this equation for $G(\ell;-\underline{m})$ in comparison to the equation for $G(\ell;\underline{m})$. It has an extra minus sign, because of the sign-factors. The first summand has one extra factor of $(-1)^{|\underline{m}|-1}$ because of the second symmetry relation of the coefficient functions F. The second summand has one extra factor of $(-1)^{|\underline{m}_1|}$ because of our induction hypothesis and one extra factor of $(-1)^{|\underline{m}_2|-1}$ because of the second symmetry relation, which is also an extra factor of $(-1)^{|\underline{m}|}$. In total, both terms have an extra factor of $(-1)^{|\underline{m}|}$, which is why equation (3.1) is the same for $G(\ell;-\underline{m})$ and $(-1)^{|\underline{m}|}G(\ell;\underline{m})$. Because the starting conditions are also the same for both functions, they are equal.

The functions G are of the form

$$G(\ell;\underline{m}) = \sum_{\nu\geq 0} Q_\nu(\ell;\underline{m})e^{-\nu\ell} \tag{3.2}$$

with non-negative integers ν and polynomials $Q_\nu(\ell;\underline{m})$ with rational coefficients, analogously to the functions f, explained in equation (2.9). Just as for those functions, the upper bound is not important to us, but it is finite. Again, we can prove equation (3.2) via induction on $|\underline{m}|$ using equation (3.1) and the starting conditions $G(0;\underline{m}) = 0$. We have already seen in section 3.1 that $G(\ell;(m_1)) = \frac{1}{m_1}\left(e^{-|m_1|\ell} - 1\right)$ for $m_1 \neq 0$ and that $G(\ell;(0)) = 0$. The former is trivially of the form described in (3.2) and the latter is also of this form with $Q_0(\ell;(m_1)) = -1$ and $Q_{|m_1|}(\ell;\underline{m}) = \frac{1}{m_1}$. This completes our base case. Our induction hypothesis is that all functions $G(\ell;\underline{m})$ with $|\underline{m}| < k$ can be written as in equation (3.2). Let $\underline{m}$ be such that $|\underline{m}| = k > 1$. According to equation (3.1), $G(\ell;\underline{m})$ is given by

$$\begin{aligned} G(\ell;\underline{m}) = &-\operatorname{sgn}(M(\underline{m}))\int F(\ell;\underline{m})\mathrm{d}\ell \\ &-\sum_{(\underline{m}_1,\underline{m}_2)=\underline{m}} \operatorname{sgn}(M(\underline{m}_2))\int G(\ell;\underline{m}_1)F(\ell;\underline{m}_2)\mathrm{d}\ell \end{aligned} \tag{3.3}$$

Because the functions $F(\ell;\underline{m}_2) = e^{-|\underline{m}_2|\ell}f(\ell;\underline{m}_2)$ are of the form (2.9) and because of our induction hypothesis, the function $G(\ell;\underline{m})$ is of the form

$$G(\ell;\underline{m}) = \sum_{\nu\geq 0} Q_\nu(\ell;\underline{m})e^{-\nu\ell} + c.$$

The starting condition implies that $c = -\sum_{\nu\geq 0} Q_\nu(0;\underline{m})$. Therefore in total, the function G is of the form

$$G(\ell;\underline{m}) = Q_0(\ell;\underline{m}) - \sum_{\nu\geq 0} Q_\nu(0;\underline{m}) + \sum_{\nu\geq 1} Q_\nu(\ell;\underline{m})e^{-\nu\ell},$$

which is again of the form stated in equation (3.2).

The coefficients $G(\infty;\underline{m})$ have to be finite for the transformation to converge. For that we have to prove that the polynomials $Q_0(\ell;\underline{m})$ are constant. This is true, because they are equal to the constant of integration from equation (3.3). Inserting $F(\ell;\underline{m}) = e^{-|M(\underline{m})|\ell}f(\ell;\underline{m})$ into this equation yields

$$\begin{aligned} G(\ell;\underline{m}) = &-\operatorname{sgn}(M(\underline{m}))\int e^{-|M(\underline{m})|\ell}f(\ell;\underline{m})\mathrm{d}\ell \\ &-\sum_{(\underline{m}_1,\underline{m}_2)=\underline{m}} \operatorname{sgn}(M(\underline{m}_2))\int G(\ell;\underline{m}_1)e^{-|M(\underline{m}_2)|\ell}f(\ell;\underline{m}_2)\mathrm{d}\ell. \end{aligned}$$

The first summand is either vanishing for $M(\underline{m}) = 0$ or exponentially decreasing for $M(\underline{m}) \neq 0$. Analogously for every breakup $(\underline{m}_1, \underline{m}_2)$ of $\underline{m}$, the second summand

is either vanishing for $M(\underline{m_2}) = 0$ or exponentially decreasing for $M(\underline{m_2}) \neq 0$. Therefore every non-vanishing integrand is exponentially decreasing and the only term contributing to $Q_0(\ell; \underline{m})$ is the integration constant.

3.3 Implementation

Because the coefficient functions G are determined by a system of recursive differential equations like the function f, the calculation is basically the same. We have to calculate the functions F first, as described in section 2.6, but we do not have to store the coefficients $F(\infty; \underline{m})$ in an extra file. Then we can once more use a loop for the order of the functions G and inside another loop for the tuples $\underline{m}$ using the mapping described in section 2.6. Because of the shape of the functions G stated in equation (3.2), they can be stored in the same way as the functions f. The arithmetic operations can be implemented as described in section 2.6. As for the functions F, the coefficients $G(\infty; \underline{m})$ can be extracted from the quasipolynomials easily, as they are given by the prefactor of the quasimonomial with $\nu = 0$.

After including all the symmetry relations from sections 2.4 and 3.2 into the program, excluding all impossible tuples and storing everything as described in section 2.6, it is possible to reach a precision of at least eleven orders when considering systems with $N = 2$ and $n \in \{-2, 0, 2\}$. The system size is not an issue for this calculation, because they are model-independent.

3.4 Results up to second order

The coefficient functions G of the unitary transformation are already much more complicated to calculate up to second order than the coefficient functions F of the Hamiltonian, calculated in section 2.7. The first order however is still easy to calculate as we saw in section 3.1. It is given by

$$\sum_{|\underline{m}|=1} G(\ell; \underline{m}) T(\underline{m}) = \sum_{n=1}^{N} \frac{1}{n} \left(e^{-n\ell} - 1 \right) (T_n - T_{-n}).$$

The effective unitary transformation up to first order is therefore given by

$$U_{(1)} = \mathbb{1} + \lambda \sum_{n=1}^{N} \frac{1}{n} (T_{-n} - T_n).$$

The second order for the coefficient functions G requires more explicit integrations than the coefficient functions F in section 2.7. That is because the coefficient functions G fulfill less symmetry relations and because they can be non-vanishing for tuples $\underline{m}$ with $|M(\underline{m})| > N$. The only factor that certainly vanishes is $G(\ell;(0,0))$, because the factor $F(\ell;(0,0))$ from equation (3.1) vanishes, as we proved in section 2.7, and because the second term vanishes due to the sign-term. All other functions do not vanish automatically and we have to compute almost all of them specifically. One of the simpler remaining functions is $G(\ell;(n,0))$ with $n > 0$, which reduces to

$$G(\ell;(n,0)) = -\int_0^\ell F(\ell';(n,0))\mathrm{d}\ell = -\int_0^\ell \ell' e^{-n\ell'}\mathrm{d}\ell = \left(\frac{\ell}{n} + \frac{1}{n^2}\right)e^{-n\ell} - \frac{1}{n^2},$$

because of the sign-term in the second summand. Using the symmetry relation from section 3.2, it also holds that

$$G(\ell;(-n,0)) = \left(\frac{\ell}{n} + \frac{1}{n^2}\right)e^{-n\ell} - \frac{1}{n^2}.$$

The function $G(\ell;(0,n))$ with $n > 0$ is equally easy to calculate, because $G(\ell;(0)) = 0$. It is given by

$$G(\ell;(0,n)) = -\int_0^\ell F(\ell';(0,n))\mathrm{d}\ell' = \int_0^\ell \ell' e^{-n\ell'}\mathrm{d}\ell' = \frac{1}{n^2} - \left(\frac{\ell}{n} + \frac{1}{n^2}\right)e^{-n\ell}.$$

This, together with the symmetry relation, yields

$$G(\ell;(0,-n)) = \frac{1}{n^2} - \left(\frac{\ell}{n} + \frac{1}{n^2}\right)e^{-n\ell}.$$

Next, we will calculate the functions $G(\ell;(n,m))$ with $n,m > 0$ arbitrary. Because $F(\ell;(n,m)) = 0$, they are given by

$$\begin{aligned} G(\ell;(n,m)) &= -\int_0^\ell G(\ell';(n))F(\ell';(m))\mathrm{d}\ell' = -\int_0^\ell \frac{1}{n}\left(e^{-(n+m)\ell'} - e^{-m\ell'}\right)\mathrm{d}\ell' \\ &= \frac{1}{n(n+m)}e^{-(n+m)\ell} - \frac{1}{nm}e^{-m\ell} + \frac{1}{m(n+m)} \end{aligned}$$

and because of the symmetry relations

$$G(\ell;(-n,-m)) = \frac{1}{n(n+m)}e^{-(n+m)\ell} - \frac{1}{nm}e^{-m\ell} + \frac{1}{m(n+m)}.$$

Because of the factor $\operatorname{sgn}(M(\underline{m}))$ in equation (3.1), the functions $G(\ell;(n,-m))$ with $n,m>0$ require case differentiation. First we will consider the case $n=m$. This yields

$$\begin{aligned} G(\ell;(n,-n)) &= \int_0^\ell G(\ell';(n))F(\ell';(-n))\mathrm{d}\ell' = \int_0^\ell \frac{1}{n}\left(e^{-2n\ell'}-e^{-n\ell'}\right) \\ &= \frac{1}{n^2}e^{-n\ell} - \frac{1}{2n^2}e^{-2n\ell} - \frac{1}{2n^2}. \end{aligned}$$

and therefore also

$$G(\ell;(-n,n)) = \frac{1}{n^2}e^{-n\ell} - \frac{1}{2n^2}e^{-2n\ell} - \frac{1}{2n^2}.$$

Next we will consider the case $n>m$. Then

$$\begin{aligned} G(\ell;(n,-m)) &= -\int_0^\ell F(\ell';(n,-m))\mathrm{d}\ell' + \int_0^\ell G(\ell';(n))F(\ell';(-m))\mathrm{d}\ell' \\ &= +\int_0^\ell \frac{1}{m}\left(e^{-(n+m)\ell'}-e^{-(n-m)\ell'}\right)\mathrm{d}\ell' + \int_0^\ell \frac{1}{n}\left(e^{-(n+m)\ell}-e^{-m\ell}\right)\mathrm{d}\ell' \\ &= -\frac{1}{m(n+m)}e^{-(n+m)\ell} + \frac{1}{m(n-m)}e^{-(n-m)\ell} + \frac{2}{n^2-m^2} \\ &- \frac{1}{n(n+m)}e^{-(n+m)\ell} + \frac{1}{nm}e^{-m\ell} + \frac{1}{m(n+m)}. \end{aligned}$$

and

$$\begin{aligned} G(\ell;(-n,m)) &= -\frac{1}{m(n+m)}e^{-(n+m)\ell} + \frac{1}{m(n-m)}e^{-(n-m)\ell} + \frac{2}{n^2-m^2} \\ &- \frac{1}{n(n+m)}e^{-(n+m)\ell} + \frac{1}{nm}e^{-m\ell} + \frac{1}{m(n+m)}. \end{aligned}$$

The case $n<m$ is analogous and yields the functions

$$\begin{aligned} G(\ell;(n,-m)) &= \frac{1}{n(n+m)}e^{-(n+m)\ell} - \frac{1}{n(m-n)}e^{-(m-n)\ell} - \frac{2}{n^2-m^2} \\ &- \frac{1}{n(n+m)}e^{-(n+m)\ell} + \frac{1}{nm}e^{-m\ell} + \frac{1}{m(n+m)} \\ G(\ell;(-n,m)) &= \frac{1}{n(n+m)}e^{-(n+m)\ell} - \frac{1}{n(m-n)}e^{-(m-n)\ell} - \frac{2}{n^2-m^2} \\ &- \frac{1}{n(n+m)}e^{-(n+m)\ell} + \frac{1}{nm}e^{-m\ell} + \frac{1}{m(n+m)}. \end{aligned}$$

Therefore the second order of the unitary transformation is given by

$$\begin{aligned}
\sum_{|\underline{m}|=2} G(\ell;\underline{m})T(\underline{m}) = &\sum_{n=1}^{N}\left(\left(\frac{\ell}{n}+\frac{1}{n^2}\right)e^{-n\ell}-\frac{1}{n^2}\right)([T_n,T_0]+[T_{-n},T_0])\\
&+\sum_{n,m=1}^{N}\left(\frac{1}{n(n+m)}e^{-(n+m)\ell}-\frac{1}{nm}e^{-m\ell}+\frac{1}{m(n+m)}\right)\\
&\qquad\times(T_nT_m+T_{-n}T_{-m})\\
&+\sum_{n=1}^{N}\left(\frac{1}{n^2}e^{-n\ell}-\frac{1}{2n^2}e^{-2n\ell}-\frac{1}{2n^2}\right)(T_nT_{-n}+T_{-n}T_n)\\
&+\sum_{n=1}^{N}\sum_{m=1}^{n-1}\Bigg(-\frac{1}{m(n+m)}e^{-(n+m)\ell}+\frac{1}{m(n-m)}e^{-(n-m)\ell}\\
&\qquad\qquad+\frac{2}{n^2-m^2}\Bigg)([T_n,T_{-m}]+[T_{-n},T_m])\\
&+\sum_{\substack{n,m=1\\ n\neq m}}^{N}\left(-\frac{1}{n(n+m)}e^{-(n+m)\ell}+\frac{1}{nm}e^{-m\ell}+\frac{1}{m(n+m)}\right)\\
&\qquad\times(T_nT_{-m}+T_{-n}T_m)
\end{aligned}$$

and the effective unitary transformation up to second order by

$$\begin{aligned}
U_{(2)} = &\mathbb{1}+\lambda\sum_{n=1}^{N}\frac{1}{n}(T_{-n}-T_n)\\
&+\lambda^2\sum_{n=1}^{N}\frac{1}{n^2}\left([T_0,T_n]+[T_0,T_{-n}]-\frac{1}{2}T_nT_{-n}-\frac{1}{2}T_{-n}T_n\right)\\
&+\lambda^2\sum_{n=1}^{N}\sum_{m=1}^{n-1}\frac{2}{n^2-m^2}([T_n,T_{-m}]+[T_{-n},T_m])\\
&+\lambda^2\sum_{\substack{n,m=1\\ n\neq m}}^{N}\frac{1}{m(n+m)}(T_nT_m+T_{-n}T_{-m}+T_nT_{-m}+T_{-n}T_m)\\
&+\lambda^2\sum_{n=1}^{N}\frac{1}{m(n+m)}(T_nT_n+T_{-n}T_{-n}) \qquad (3.4)
\end{aligned}$$

These two rather complicated expressions emphasize the utility of computer aided calculations.

4 Toric Code

The toric code is a theoretical model introduced by Kitaev in 1997 in [3]. It is an exactly solvable model that realizes topological order and anyonic excitations. The eigenstates of the Hamiltonian are highly entangled.

4.1 Definition

The toric code can be defined for several different lattices. We will pick the one illustrated in figure 4.1. It is a two-dimensional $N \times N$ square lattice with periodic boundary conditions and one spin-$\frac{1}{2}$ particle for every one of the $2N^2$ edges. Therefore, the total Hilbert space is a tensor product of $2N^2$ single particle Hilbert spaces and has dimension 2^{2N^2}. The spin-$\frac{1}{2}$ particles will be referred to as spins from now on. Please note that the N here is not the same as in chapter 2.

There are two kinds of operators in the toric code Hamiltonian – the star operators and the plaquette operators. Operators from both types act on four spins each, which is illustrated in figure 4.1. We introduce a star operator for every vertex and a plaquette operator for every face of the lattice. The operators are defined by

$$A_s = \prod_{i \in s} \sigma_i^x, \qquad B_p = \prod_{i \in p} \sigma_i^z,$$

where $i \in s$ denotes the four spins closest to the vertex s and $i \in p$ the four spins adjacent to the face p. The overall Hamiltonian is

$$H = -\frac{1}{2} \sum_{\text{stars } s} A_s - \frac{1}{2} \sum_{\text{plaquettes } p} B_p. \tag{4.1}$$

In total the Hamiltonian contains N^2 operators of each type, because the lattice consists of N^2 vertices and N^2 faces.

As the basic building block of the Hamiltonian, it is worth mentioning the semantics of the operators σ_i^x and σ_i^z. σ_i^x acts as a Pauli x matrix on the i-th particle and as

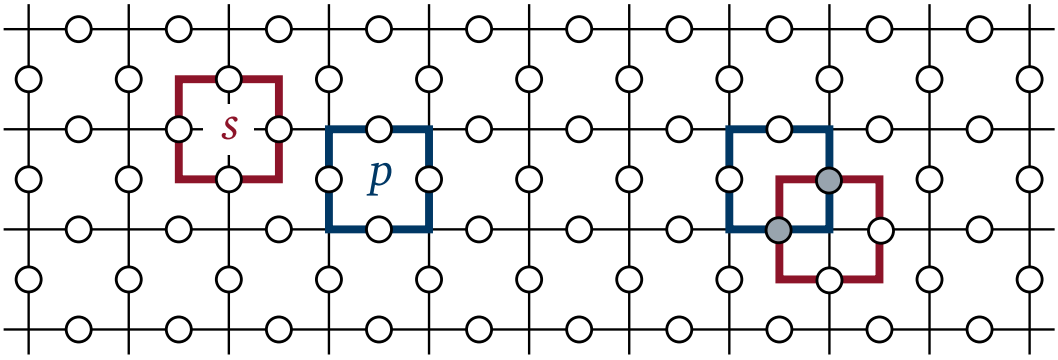

Abbildung 4.1: The lattice of the toric code is a two-dimensional square lattice with periodic boundary conditions. The circles represent spin-$\frac{1}{2}$ particles sitting on the edges. The red squares represent star operators, the blue ones plaquette operators. Every pair consisting of one star and one plaquette operator either has no or two spins in common. The left operators share no spins, the right operators share the spins marked in grey.

unity on the other particles. More precisely, it is the tensor product of $2N^2 - 1$ unity matrices and one Pauli x matrix defined as

$$\sigma_i^x := \mathbb{1}_2 \otimes \ldots \otimes \mathbb{1}_2 \otimes \underset{\substack{\uparrow \\ i}}{\sigma^x} \otimes \mathbb{1}_2 \otimes \ldots \otimes \mathbb{1}_2,$$

where the σ^x is at the i-th position. Analogously, σ_i^z is defined as

$$\sigma_i^z := \mathbb{1}_2 \otimes \ldots \otimes \mathbb{1}_2 \otimes \underset{\substack{\uparrow \\ i}}{\sigma^z} \otimes \mathbb{1}_2 \otimes \ldots \otimes \mathbb{1}_2.$$

Defining the Pauli matrices like this ensures that two operators acting on different spins commute automatically.

For this reason, the star and plaquette operators are their own inverse. This can be calculated via

$$A_s^2 = \prod_{i \in s} (\sigma_i^x)^2 = \mathbb{1}, \qquad B_p^2 = \prod_{i \in p} (\sigma_i^z)^2 = \mathbb{1},$$

where $\mathbb{1} := \mathbb{1}_2 \otimes \ldots \otimes \mathbb{1}_2$. As products of Pauli matrices the star and plaquette operators have the two eigenvalues 1 and -1.

4.2 Complete set of commuting observables

We will use observables and their eigenvalues to describe states of our system. The important notion in this context is the complete set of commuting observables (CSCO). The paragraphs cited in this section are from chapter II of [11].

Since observables are Hermitian operators, their eigensubspaces are orthogonal to each other, which is shown in § D-2. Because every state can be normalized, we can find an orthonormal basis of eigenstates for every observable. If two observables commute, we can use one fundamental result from § D-3-a, namely that we can always find an orthonormal basis of eigenstates common to both observables. Iteratively, we can find an orthonormal basis of eigenstates common to more than two commuting observables. Keeping this in mind, we can define a CSCO as in § D-3-b:

> A set of observables [...] is a complete set of commuting observables if there exists a unique orthonormal basis of common eigenvectors [...].

It is always possible to extend a given set of commuting observables to a CSCO. Using the eigenstates of one observable as basis, this observable is diagonal. Using the eigenstates of a CSCO as basis, every observable in that CSCO is diagonal.

CSCOs for the toric code model would be for example all the Pauli x matrices or all the Pauli z matrices. To describe time-independent states, we want a CSCO whose observables also commute with the Hamiltonian given in equation (4.1). This is why the aforementioned examples are not suitable for us. It is natural to consider the star and plaquette operators, because the Hamiltonian is composed of these operators. A CSCO containing all star and plaquette operators would generate a time-independent eigenbasis with respect to which the Hamiltonian is diagonal.

The first question is whether this set of observables is a set of commuting observables. This can immediately be seen for two star or two plaquette operators, because they consist of the same type of Pauli matrix and commute trivially. One star and one plaquette operator also commute, because they either have no or two spins in common, which is illustrated in figure 4.1. The pairs that share no spins commute automatically, because Pauli matrices acting on different spins commute automatically. The case where a star and a plaquette operator share two spins requires a short consideration. Recall that $\sigma^x\sigma^z = -\sigma^z\sigma^x$. For $i \neq j$ it holds that

$$[\sigma_i^x\sigma_j^x, \sigma_i^z\sigma_j^z] = \sigma_i^x\sigma_i^z\sigma_j^x\sigma_j^z - \sigma_i^z\sigma_i^x\sigma_j^z\sigma_j^x = \sigma_i^x\sigma_i^z\sigma_j^x\sigma_j^z - (-\sigma_i^x\sigma_i^z)(-\sigma_j^x\sigma_j^z) = 0,$$

and the operators sharing exactly the two spins i and j commute. This result can also be generalized. Every product of Pauli x matrices commutes with every product of Pauli z matrices if they share an even number of spins. Because of this, the star and plaquette operators commute with each other and with the overall Hamiltonian, which makes them suitable for a CSCO.

The second question is whether the set of commuting observables is complete. The Hilbert space has dimension 2^{2N^2}. So far, we only considered observables with two

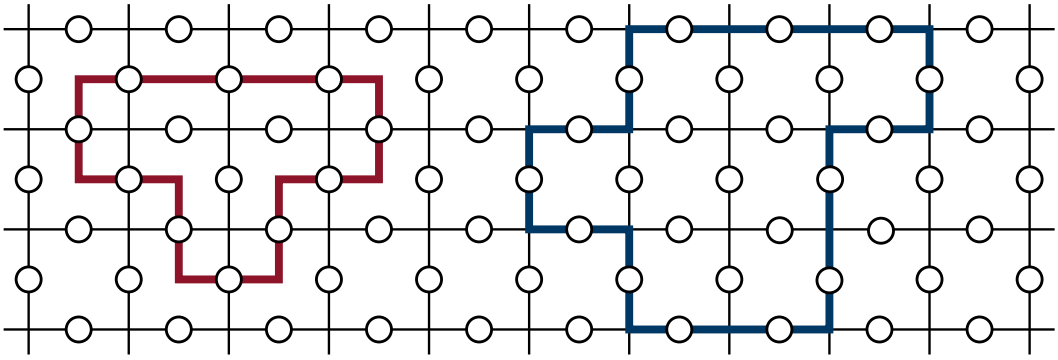

Abbildung 4.2: The red and blue contractible loops displayed here are examples for operators that commute with the Hamiltonian. The red loop, that is located on the dual lattice, is a product of Pauli x matrices, the blue one, located on the lattice, a product of Pauli z matrices. Both loops can also be written as products of star and plaquette operators. The red loop can be written as the product of all star operators within it and the blue one as the product of all plaquette operators within it.

distinct eigenvalues each. This implies that for a CSCO, we need in total $2N^2$ of these observables and they have to be independent, i.e. every combination of their $2N^2$ eigenvalues has to fit one eigenstate.

Because of the periodic boundary conditions it holds that

$$\prod_{\text{stars } s} A_s = \prod_{\text{spins } i} (\sigma_i^x)^2 = \mathbb{1}, \qquad \prod_{\text{plaquettes } p} B_p = \prod_{\text{spins } i} (\sigma_i^z)^2 = \mathbb{1}. \tag{4.2}$$

For every eigenstate, the number of star operators that have eigenvalue -1 has to be even and so does the number of plaquette operators with eigenvalue -1. This leaves one star and one plaquette operator dependent on the others. At least two new operators are needed to form a CSCO. The new operators should be composed out of Pauli matrices, because they have to contain information about the spins. There are some restrictions on how to do this, because arbitrary products of Pauli matrices do not necessarily commute with every star and plaquette operator.

Let us consider loops like in figure 4.2. They represent products of Pauli matrices along the red line that is located on the dual lattice or along the blue line that is located on the lattice. One loop must not contain different types of Pauli matrices, because it would not commute with all the star and plaquette operators. Let us have a closer look at the red loop. Regardless of the type of Pauli matrix we choose for the loop, it will commute with every plaquette operator, because they share an even number of links. It also commutes with every star operator if the loop consist of Pauli x matrices. Then it will also commute with the Hamiltonian. Analogously we can examine the blue loop and come to the conclusion, that it commutes with every star and plaquette operator and with the Hamiltonian if it consists of Pauli z matrices.

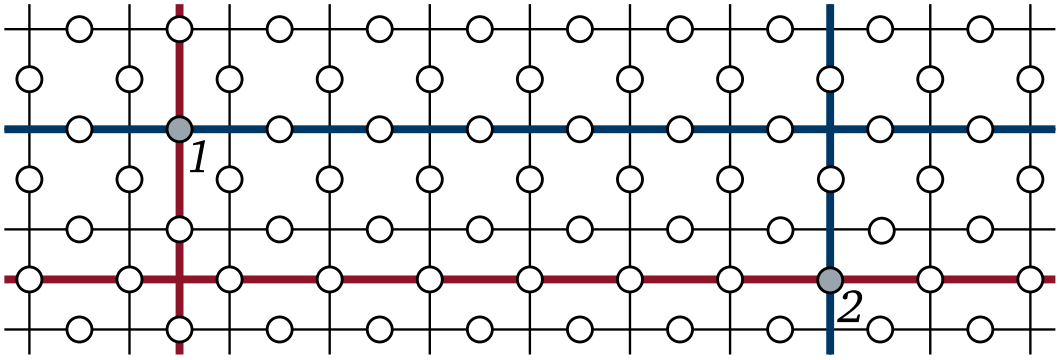

Abbildung 4.3: There are four types of non-contractible loops illustrated here. The red lines on the dual lattice represent products of Pauli x matrices, the blue ones on the lattice represent products of Pauli z matrices. The red loops commute with one another, so do the blue loops. Parallel red and blue loops also commute with one another, because they do not share any spins. A red and a blue loop perpendicular to one another do not commute, because they have exactly one spin in common. The respective spins are marked grey and labeled by 1 and 2. Spin 1 is located on a horizontal bond and the spin 2 on a vertical bond.

Every other loop constructed like the two loops in figure 4.2 also commutes with every one of the operators. Let us look at the red loop again. Because the loop is a product of Pauli x matrices and because of $(\sigma^x)^2 = \mathbb{1}_2$, the loop is the product of all the star operators enclosed by it. The same holds for the blue loop that is a product of all the plaquette operators enclosed by it. They are therefore not independent from the star and plaquette operators, because their eigenvalue is the product of the eigenvalues of the enclosed operators.

On a torus, there are also non-contractible loops like the ones illustrated in figure 4.3. As they are loops, they also commute with every star and every plaquette operator with the same arguments as for the contractible loops. It is possible to generate an even number of non-contractible loops using products of star or plaquette operators, but it is not possible to generate just one non-contractible loop in this way. Every single non-contractible loop is independent of all the star and plaquette operators. They may however depend on one another or on a combination of non-contractible loops and star and plaquette operators.

We will denote the red loops, that consist of Pauli x matrices, by X and the blue loops by Z. More specifically, the loops that contain the spin marked 1 will be denoted by X_1 and Z_1 and the loops that contain spin 2 are X_2 and Z_2. Please note that the choice of spin 1 and 2 is arbitrary as long as one of them is located on a horizontal and the other one on a vertical bond. Let us look at X_1 and X_2. Every other non-contractible red loop imaginable is depending on these two loops and the star operators, because we can use star operators to deform X_1 and X_2. Analogously,

every other non-contractible blue loop is depending on Z_1 and Z_2 and the plaquette operators.

Therefore it suffices to examine the aforementioned four loops containing spin 1 and 2. We cannot choose the pair X_1 and Z_1 because they anti-commute, as they only share spin 1. Likewise we cannot choose X_2 and Z_2. Let us, without loss of generality, pick the loop X_1. Now we could either extend our choice by X_2 or by Z_2. It does not matter which operator we choose, because both of them are independent of X_1 and of all the star and plaquette operators. We will choose without loss of generality the loop X_2. Both loops have the eigenvalues 1 and -1.

We have not ruled out more constraints as the two in equation (4.2) yet, but we can motivate that there are no more. Let us consider for a moment that there is another constraint. This would make another one of the $2N^2$ remaining operators in our set dependent on the others. We would find another observable to complete our CSCO, but there are no more possibilities left. The only products of Pauli matrices that commute with all star and plaquette operators and our two non-contractible loops are loops, but we already included or ruled out every possible loop. This implies that our set is a complete set and we found our CSCO.

The fact that there are loops that cannot be written in terms of operators from the Hamiltonian because of the topology of the underlying lattice is the reason for the topological order of the toric code.

4.3 Spectrum

Let us have a look at the ground states of the Hamiltonian given in equation (4.1). The eigenvalues of the star and plaquette operators corresponding to a ground state are 1. The eigenvalues of the loop operators do not affect the energy of a state. The ground-state manifold is therefore fourfold degenerate. All ground states have the energy $-N^2$ and the spectrum is bounded from below. The states with the highest energy are eigenstates corresponding to the eigenvalues -1 of the star and plaquette operators. Their energy is N^2. Because of condition (4.2) it holds that for every eigenstate the number of star or plaquette operators with eigenvalue -1 corresponding to that state has to be even. Therefore the spectrum is equidistant with energy difference $\Delta E = 2$ between two energy eigenvalues.

4.4 Ground-state manifold

The ground states are easy to find in the basis generated by our CSCO. Every ground state is a superposition of the four eigenstates corresponding to the eigenvalues -1 of all star and plaquette operators. The eigenvalues of the loop operators do not affect the energy of a state, which is why there are four eigenstates with the lowest energy. It is not immediately clear what the ground states look like in the eigenbasis of the Pauli matrices of one type. Without loss of generality, we will consider Pauli z matrices.

We will start with the state $|\Uparrow\rangle$. It is the unique eigenstate to all the Pauli z matrices that corresponds to eigenvalue 1. It is also an eigenstate to all the plaquette operators corresponding to eigenvalue 1. To convert it to a state that is also eigenstate to all the star operators, we can use projectors. If we have an arbitrary state and we want to project it onto an eigenstate of the star operator A_s corresponding to eigenvalue ± 1, we can use the projector $\frac{1}{2}(A_s \pm 1)$. This is a projector because

$$\left(\frac{1}{2}(A_s \pm 1)\right)^2 = \frac{1}{4}(A_s^2 \pm 2A_s + 1) = \frac{1}{4}(1 \pm 2A_s + 1) = \frac{1}{2}(A_s \pm 1).$$

To project our soon to be ground state, we use more of these projectors and end up with the state

$$\left(\prod_{\text{stars } s} \frac{1}{2}(A_s + 1)\right) |\Uparrow\rangle .$$

This is a ground state, but not one of the basis states of our CSCO, because it is not an eigenstate to the loop operators.

If we wanted to take an arbitrary state and project it onto the ground-state manifold we would have to use additional projectors for the plaquettes. We could even select one of the four basis states in the ground-state manifold by including projectors for the loop operators. The four basis states of the ground-state manifold are given by

$$|0; \pm 1, \pm 1\rangle = \frac{1}{2}(X_1 \pm 1)\frac{1}{2}(X_2 \pm 1) \left(\prod_{\text{plaquettes } p} \frac{1}{2}(B_p + 1)\right) \left(\prod_{\text{stars } s} \frac{1}{2}(A_s + 1)\right) |\Uparrow\rangle$$

Because all of our operators commute with each other, the order of the projections does not matter. The choice of the value ± 1 however does matter, as it selects one of the four possible basis states.

We can now see that our ground state looks very complicated using the eigenbasis of the Pauli z matrices. Since every loop on the dual lattice that is a product of Pauli

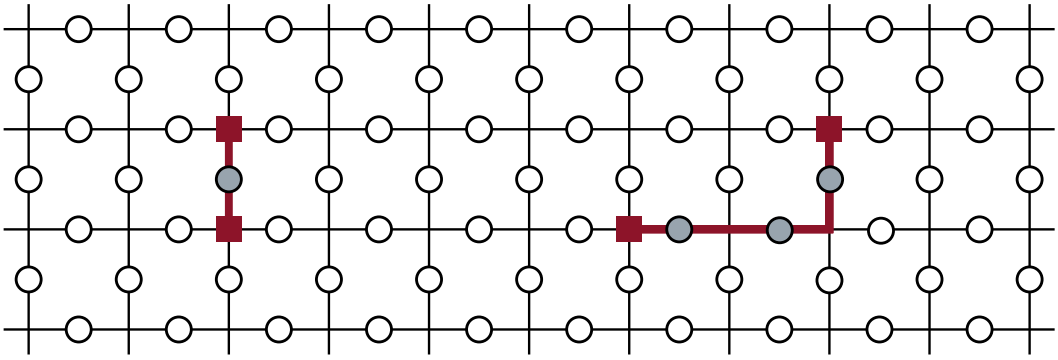

Abbildung 4.4: The red squares denote star operators with eigenvalue -1. The star operators of all the other vertices have eigenvalue 1. This state can achieved by the action of one Pauli z matrix for every grey spin on the state $|0;1,1\rangle$.

x matrices can be written as product of star and loop operators and since every product of star and loop operators is a product of loops on the dual lattice, it holds that our ground state $|0;1,1\rangle$ is a superposition of equal weights of all possibilities to flip spins of $|\Uparrow\rangle$ along loops on the dual lattice. This is a highly entangled state often called loop soup.

The loop operators Z_1 and Z_2 that we have not chosen for our CSCO can be used to switch from one basis state of the ground-state manifold to another. Using that Z_1 antikommutes with X_1 and commutes with every other operator in our CSCO, it holds that

$$\begin{aligned} -Z_1|0;1,1\rangle &= \frac{1}{2}(-Z_1X_1 \mp Z_1)\frac{1}{2}(X_2 \pm 1)\left(\prod_{\text{stars } s}\frac{1}{2}(A_s+1)\right)|\Uparrow\rangle \\ &= \frac{1}{2}(X_1Z_1 \mp Z_1)\frac{1}{2}(X_2 \pm 1)\left(\prod_{\text{stars } s}\frac{1}{2}(A_s+1)\right)|\Uparrow\rangle \\ &= \frac{1}{2}(X_1 \mp 1)\frac{1}{2}(X_2 \pm 1)\left(\prod_{\text{stars } s}\frac{1}{2}(A_s+1)\right)|\Uparrow\rangle = |0;-1,1\rangle\,. \end{aligned}$$

Analogously, it holds that $-Z_2|0;1,1\rangle = |0;1,-1\rangle$ and that $Z_1Z_2|0;1,1\rangle = |0;-1,-1\rangle$.

4.5 Excitations

The conditions from equation (4.2) prevent states corresponding to eigenvalue -1 for exactly one star or one plaquette operator. For simplicity, we will only consider eigenstates to eigenvalue 1 for all plaquette operators. The first excited states correspond to eigenvalue -1 for exactly two star operators. We will see that the relative positions of the two star operators do not matter, every combination is possible. But first let us have a look at figure 4.4. All star operators in this figure have eigenvalue 1 except for the ones represented by a red square. The grey spins mark

possible paths from one of these star operators to another. The desired eigenvalues of the star operators are achieved via action of Pauli z matrices. Let us denote the spin on the left side of figure 4.4 by i and the two adjacent star operators by s_1 and s_2. Using that $\sigma_i^z A_{s_j} = -A_{s_j}\sigma_i^z$, it holds that

$$\begin{aligned}|s_1, s_2; 1, 1\rangle := \sigma_i^z \,|0; 1, 1\rangle &= \sigma_i^z \left(\prod_{\text{stars } s} \frac{1}{2}(A_s + 1)\right) |\Uparrow\rangle \\ &= \left(\prod_{\text{stars } s \neq s_1, s_2} \frac{1}{2}(A_s + 1)\right) \frac{1}{2}(A_{s_1} - 1)\frac{1}{2}(A_{s_2} - 1)\,|\Uparrow\rangle\,.\end{aligned}$$

The state $|s_1, s_2\rangle$ is the eigenstate corresponding to eigenvalue 1 for all operators except for the two star operators A_{s_1} and A_{s_2}. Analogously, we can generate the excitation on the right side of figure 4.4 by acting on $|0; 1, 1\rangle$ with one Pauli z matrix for every grey spin. The exact path of Pauli z matrices for an excitation is arbitrary, because the star operators that are not at the end points of the path are not affected. Because of that, the notation $|s_1, s_2; 1, 1\rangle$ is well-defined and we will use it from now on for every excited state.

We can also use excitations to switch from one ground state to another, for example from $|0; 1, 1\rangle$ to $|0; -1, 1\rangle = -Z_1\,|0; 1, 1\rangle$ by an energy cost of 2. The energy is needed to change the eigenvalue of two adjacent star operators to -1 using one of the Pauli z matrices from Z_1. Then we use more Pauli z matrices to move the excitation around the torus along Z_1 and to annihilate them again. The result is the same as acting directly with Z_1.

If we drop the simplification of regarding only states corresponding to eigenvalue 1 for the plaquette operators, then we can also generate plaquette excitations and move them around. An interesting feature arises. The different excitations pick up a phase if wound around each other. This means that the toric code realizes mutual anyonic statistic. We will not go into that further.

5 Toric Code in a low magnetic field

We switch on a low magnetic field in z-direction. The new Hamiltonian is

$$H = -\frac{1}{2}\sum_{\text{stars } s} A_s - \frac{1}{2}\sum_{\text{plaquettes } p} B_p + \lambda \sum_{\text{spins } i} \sigma_i^z.$$

We already saw that the spectrum of the unperturbed toric code Hamiltonian is equidistant and bounded from below.

The eigenvalues of eigenstates of the plaquette operators are conserved, because the plaquette operators commute with the perturbation and therefore with the whole Hamiltonian. We only consider states where these eigenvalues are 1, because we are interested in low energy solutions and do not want to pay attention to the anyonic statistics mentioned in section 4.5.

The Hamiltonian then reduces to

$$\begin{aligned} H &= -\frac{N^2}{2} - \frac{1}{2}\sum_{\text{stars } s} A_s + \lambda \sum_{\text{spins } i} \sigma_i^z \\ &= -N^2 - \frac{1}{2}\sum_{\text{stars } s} (A_s - 1) + \lambda \sum_{\text{spins } i} \sigma_i^z = H_0 + \lambda \sum_{\text{spins } i} \sigma_i^z. \end{aligned} \tag{5.1}$$

To use the pCUT formalism introduced in the chapters 2 and 3, it is useful to rewrite the reduced Hamiltonian using second quantization.

5.1 Second quantization

Let us introduce the creation and the annihilation operators by defining their action on our eigenstates. Eigenstates of the star operator A_s corresponding to eigenvalue 1 vanish after the annihilation operator b_s acts on them. Acting with the creation operator $b_s^\dagger$ instead results in another eigenstate corresponding to eigenvalue -1 instead, while all other eigenvalues remain untouched. Analogously, eigenstates corresponding to eigenvalue -1 vanish after the creation operator $b_s^\dagger$ acts on them and become eigenstates corresponding to eigenvalue 1 after the annihilation operator b_s acts on them.

Observe that $-\frac{1}{2}(A_s - 1)$ projects an eigenstate onto itself if the corresponding eigenvalue is -1 and causes the state to vanish if the eigenvalue is 1. In other words, it "counts" if the state is excited. In terms of the creation and annihilation operators it can be written as the number operator $n_s := b_s^\dagger b_s = -\frac{1}{2}(A_s - 1)$. The converse of this definition is $A_s = 1 - 2n_s$.

This relation can be used to calculate the commutation relations of the creation and annihilation operators. Because these operators either cause the state to vanish, or change exactly one eigenvalue and act as the identity on all the others, they automatically commute when acting on different eigenvalues. The only interesting case left is $[b_s^\dagger, b_s] = b_s^\dagger b_s - b_s b_s^\dagger$. If an eigenstate of A_s has eigenvalue 1, then it is also an eigenstate of $[b_s^\dagger, b_s]$ corresponding to the same eigenvalue because of the first summand. If the eigenstate of A_s has eigenvalue -1, then it is also an eigenstate of $[b_s^\dagger, b_s]$ also corresponding to the eigenvalue -1 because of the second summand. Therefore it holds that $[b_s^\dagger, b_s] = A_s = 1 - 2n_s$ and the quasi-particles behave like hard-core bosons.

In the eigenbasis of the Pauli z matrices, an arbitrary eigenstate of H_0 is given by

$$|\psi\rangle = \left(\prod_{\text{stars } s} \frac{1}{2}(A_s \pm 1) \right) |\Uparrow\rangle$$

with $\pm$ chosen almost arbitrarily for every operator. Because of the conditions in equation (4.2) the number of times we choose the minus sign has to be even. We already saw that $\sigma_i^z A_s = -A_s \sigma_i^z$ for a star operator A_s that affects the spin i. This implies $\sigma_i^z (A_s \pm 1) = -(A_s \mp 1)\sigma_i^z$, and therefore the perturbation flips the eigenvalues of the two adjacent star operators. Depending on the eigenvalues of these operators, the perturbation either lowers or raises the energy by 1, or swaps the eigenvalues of two adjacent star operators. In terms of the creation and annihilation operators this can be written as

$$\sigma_i^z = b_{s_1} b_{s_2} + b_{s_1} b_{s_2}^\dagger + b_{s_1}^\dagger b_{s_2} + b_{s_1}^\dagger b_{s_2}^\dagger,$$

where A_{s_1} and A_{s_2} are the two star operators that affect the spin i.

In total, the Hamiltonian from equation (5.1) can be rewritten as

$$\begin{aligned} H = -N^2 + \sum_{\text{stars } s} n_s + \lambda \sum_{\text{stars } s} \Big(& b_s b_{s+e_1} + b_s b_{s+e_2} + b_s^\dagger b_{s+e_1}^\dagger + b_s^\dagger b_{s+e_2}^\dagger \\ & + b_s b_{s+e_1}^\dagger + b_s^\dagger b_{s+e_1} + b_s b_{s+e_2}^\dagger + b_s^\dagger b_{s+e_2} \Big). \end{aligned}$$

where e_j is an abbreviation for the next neighbour in the horizontal or vertical direction.

5.2 pCUT results up to second order

Now we can define the operators needed for the pCUT formalism

$$\begin{aligned} T_{-2} &:= \sum_{\text{stars } s} (b_s b_{s+e_1} + b_s b_{s+e_2}) \\ T_0 &:= \sum_{\text{stars } s} (b_s b^\dagger_{s+e_1} + b^\dagger_s b_{s+e_1} + b_s b^\dagger_{s+e_2} + b^\dagger_s b_{s+e_2}) \\ T_2 &:= \sum_{\text{stars } s} (b^\dagger_s b^\dagger_{s+e_1} + b^\dagger_s b^\dagger_{s+e_2}) \end{aligned}$$

and write the Hamiltonian from equation (5.1) as

$$H = -N^2 + \sum_{\text{stars } s} n_s + \lambda(T_{-2} + T_0 + T_2).$$

Therefore we can apply the pCUT formalism from chapters 2 and 3.

As an example, the non-vanishing coefficient functions from the calculations up to second order in section 2.7 are

$$\begin{aligned} F(\ell;(-2)) &= e^{-2\ell} & F(\ell;(0)) &= 1 & F(\ell;(2)) &= e^{-2\ell} \\ F(\ell;(0,-2)) &= \ell e^{-2\ell} & F(\ell;(2,-2)) &= \frac{1}{2}\left(1-e^{-4\ell}\right) & F(\ell;(2,0)) &= \ell e^{-2\ell} \\ F(\ell;(-2,0)) &= -\ell e^{-2\ell} & F(\ell;(-2,2)) &= -\frac{1}{2}\left(1-e^{-4\ell}\right) & F(\ell;(0,2)) &= -\ell e^{-2\ell} \end{aligned}$$

and the effective Hamiltonian is

$$H^{(2)}_{\text{eff}} = -N^2 + \sum_{\text{stars } s} n_s + \lambda T_0 + \frac{\lambda^2}{2}[T_2, T_{-2}]. \tag{5.2}$$

The non-vanishing coefficient functions from the calculations up to second order in section 3.4 are

$$\begin{aligned} G(\ell;(-2)) &= \frac{1}{2}\left(1-e^{-2\ell}\right) & G(\ell;(2)) &= -\frac{1}{2}\left(1-e^{-2\ell}\right) \\ G(\ell;(0,-2)) &= \frac{1}{4}\left(1-(1+2\ell)e^{-2\ell}\right) & G(\ell;(0,2)) &= \frac{1}{4}\left(1-(1+2\ell)e^{-2\ell}\right) \\ G(\ell;(-2,0)) &= -\frac{1}{4}\left(1-(1+2\ell)e^{-2\ell}\right) & G(\ell;(2,0)) &= -\frac{1}{4}\left(1-(1+2\ell)e^{-2\ell}\right) \\ G(\ell;(-2,-2)) &= \frac{1}{8}\left(1-2e^{-2\ell}+e^{-4\ell}\right) & G(\ell;(2,2)) &= \frac{1}{8}\left(1-2e^{-2\ell}+e^{-4\ell}\right) \\ G(\ell;(-2,2)) &= -\frac{1}{8}\left(1-2e^{-2\ell}+e^{-4\ell}\right) & G(\ell;(2,-2)) &= -\frac{1}{8}\left(1-2e^{-2\ell}+e^{-4\ell}\right) \end{aligned}$$

and the effective unitary transformation is

$$U_{(2)} = \mathbb{1} + \frac{\lambda}{2}(T_{-2} - T_2) + \frac{\lambda^2}{4}([T_0, T_{-2}] + [T_0, T_2]) + \frac{\lambda^2}{8}(T_{-2}T_{-2} + T_2T_2 - T_{-2}T_2 - T_2T_{-2}).$$

It is very easy to calculate that this transformation is in fact unitary up to second order. One possible check for the correctness of the algorithm is $U_{(2)}^\dagger H U_{(2)} = H_{\text{eff}}^{(2)}$. Another test is to calculate whether the transformed vectors are still normalized. We will not perform any of these tests explicitly here, as the calculations become very long for higher orders.

5.3 Applications

Possible applications of the pCUT formalism described in chapter 2 are calculations that explicitly require the Hamiltonian. As examples, we will calculate the energy of the transformed ground state $U_{(2)} |0;1,1\rangle$ and the evolution of the excited state $|s, s+e_1;1,1\rangle$.

Using the definitions of T_{-2} and T_2, the energy of the transformed ground state $U_{(2)} |0;1,1\rangle$ can be calculated by

$$\begin{aligned}
&\langle 0;1,1| U_{(2)}^\dagger H U_{(2)} |0;1,1\rangle = \langle 0;1,1| H_{\text{eff}}^{(2)} |0;1,1\rangle = -N^2 - \frac{\lambda^2}{2} \langle 0;1,1| T_{-2}T_2 |0;1,1\rangle \\
&= -N^2 - \frac{\lambda^2}{2} \sum_{\text{stars } s,t} \langle 0;1,1| (b_s b_{s+e_1} + b_s b_{s+e_2})(|t, t+e_1;1,1\rangle + |t, t+e_2;1,1\rangle) \\
&= -N^2 - \frac{\lambda^2}{2} \sum_{\text{stars } s,t} (\langle 0;1,1| b_s b_{s+e_1} |t, t+e_1;1,1\rangle + \langle 0;1,1| b_s b_{s+e_2} |t, t+e_2;1,1\rangle) \\
&= -N^2 - \frac{\lambda^2}{2} \sum_{\text{stars } s,t} 2\delta_{s,t} \langle 0;1,1|0;1,1\rangle = -N^2 - \lambda^2 \sum_{\text{stars } s} 1 = -N^2 - \lambda^2 N^2
\end{aligned}$$

Setting $\lambda = 0$ yields $\langle 0;1,1| H_0 |0;1,1\rangle = -N^2$, which is one of our results from section 4.3. Calculations like this one can be used to keep track of the behaviour of eigenstates while tuning a magnetic field. This is one possibility to investigate phase transitions.

Calculating the action of the effective Hamiltonian on certain states can enhance the understanding of the system. We will, as an example, consider the state $|s, s+e_1;1,1\rangle$ depicted in the upper picture in figure 5.1. As an excited state, it

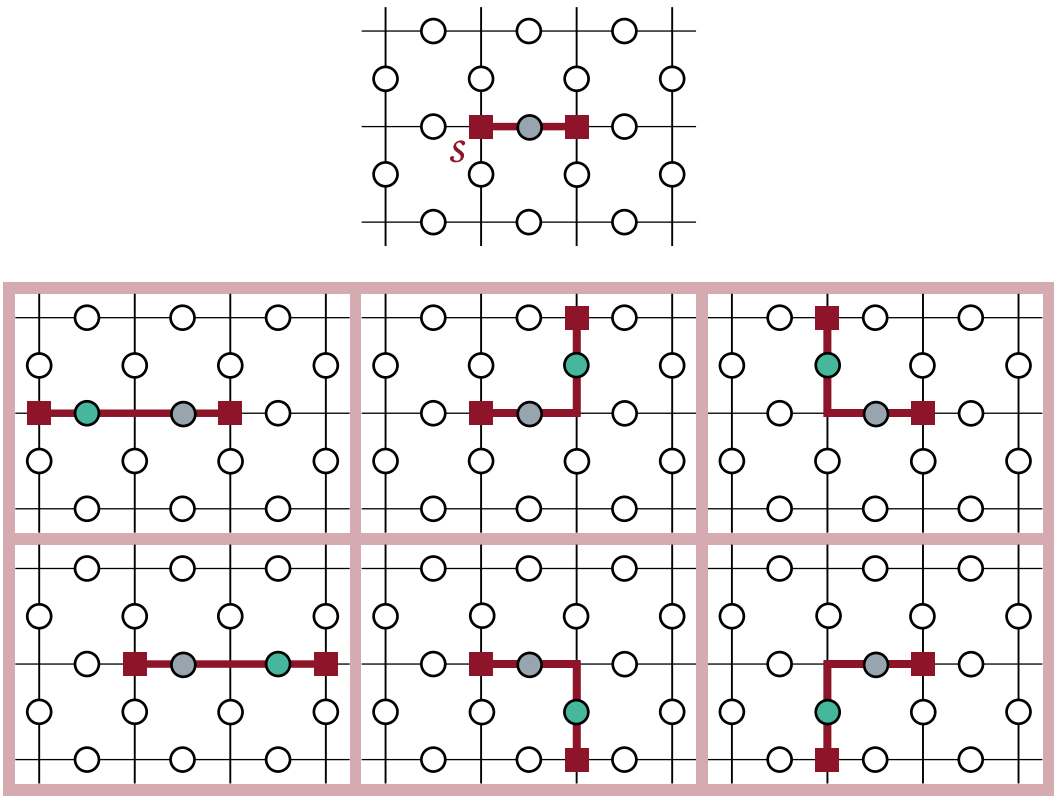

Abbildung 5.1: The upper picture represents the state $|s, s+e_1; 1, 1\rangle = b_s^\dagger b_{s+e_1}^\dagger |0; 1, 1\rangle$. The state $T_0 |s, s+e_1; 1, 1\rangle$ is represented in the lower six pictures. It contains six summands, each depicted in one image. The red background indicates, that the state is a superposition of the summands with prefactor $+1$. The grey spin is the same spin as in the upper picture. The green spins represent the action of T_0. The energy of both states is the same, T_0 just moves the excitation one step. Because of the symmetries of the underlying lattice, every horizontal and vertical flip of an upcoming term is also a term of the result.

will help us understand different properties of our perturbed system. Our goal is to calculate

$$\left(-N^2 + \sum_{\text{stars } s} n_s + \lambda T_0 + \frac{\lambda^2}{2}[T_2, T_{-2}]\right) |s, s+e_1; 1, 1\rangle \,.$$

The zeroth order is easy to calculate, it is given by

$$\left(-N^2 + \sum_{\text{stars } s} n_s\right) |s, s+e_1; 1, 1\rangle = (-N^2 + 2) |s, s+e_1; 1, 1\rangle \,.$$

The first order requires more calculation. It is given by

$$\begin{aligned} T_0 |s, s+e_1; 1, 1\rangle &= \sum_{\text{stars } t} \left(b_{t+e_1}^\dagger b_t + b_t^\dagger b_{t+e_1} + b_{t+e_2}^\dagger b_t + b_t^\dagger b_{t+e_2}\right) |s, s+e_1; 1, 1\rangle \\ &= |s-e_1, s+e_1; 1, 1\rangle + |s, s+e_1+e_2; 1, 1\rangle + |s+e_2, s+e_1; 1, 1\rangle \\ &\quad + |s, s+2e_1; 1, 1\rangle + |s, s+e_1-e_2; 1, 1\rangle + |s-e_2, s+e_1; 1, 1\rangle \,. \end{aligned}$$

This calculation is not too difficult, but one can also develop an intuition for the result without explicitly calculating it. Have a look at figure 5.1. The upper picture represents the state $|s, s+e_1; 1, 1\rangle$, the six pictures below represent the six summands we just calculated. Unsurprisingly, the action of T_0 moves the excitations around in a local manner. In a similar way, it is possible to think of the results of $[T_2, T_{-2}]\,|s, s+\delta_1; 1, 1\rangle$. Because of the commutator, only creation and annihilation operations that do not commute remain. The resulting state is depicted in figure 5.2. The action of the operator $[T_2, T_{-2}]$ also moves the excitations around in a local manner. In some contributions, one excitation moves two places further, in some contributions, both excitations move one place further. There are also contributions that are constant, because the creation and annihilation operator can act on the same spin. This type of calculations can be used to calculate all the matrix elements in the different quasi-particle blocks of the Hamiltonian and to diagonalize the blocks afterwards.

There are also applications of the pCUT formalism that require the calculations from chapter 3, for example regarding general observables. When calculating matrix elements of the observable O, it is possible to calculate the effective observable $O_{\text{eff}} = U_{\text{eff}}^{\dagger} O U_{\text{eff}}$ directly in a similar manner to the calculations described in chapters 2 and 3. This yields in general a very complicated matrix representation using a rather simple basis. Instead, one could also transform the basis states using the unitary transformation from chapter 3 and the matrix representation becomes less complicated. This is also convenient when calculating several observables.

One interesting observable regarding the toric code in the presence of a magnetic field is the loop operator Z_1. We saw in section 4.4 that the ground-state manifold is four-fold degenerate. The four basis states of the ground-state manifold can be labeled using the eigenvalues of the two loop operators X_1 and X_2. It is possible to switch between them using the two loop operators Z_1 and Z_2. The question now is whether the magnetic field is also able to switch between the ground-state basis states. For every order k in our perturbative calculation the perturbation is able to act with k Pauli z matrices. Therefore a low magnetic field cannot switch between the ground-state basis states when the system is infinitely large, because then the loop operator Z_1 is composed out of infinitely many Pauli z matrices. Thus the ground states of an infinitely large system are stable with respect to the perturbation of our magnetic field. We can also calculate which order of the magnetic field is necessary to switch between the ground-state basis states when the system size is finite. We know that the order of the magnetic field has to be at least N, because Z_1 consists of N Pauli z matrices. Because of computational limits it is hard to calculate the perturbed basis states for high orders of the magnetic field, since the number of terms needed for one basis state increases exponentially. It is also computationally more challenging to calculate the basis states for large systems, since the dimension

of the Hilbert space is equal to the number of spins. The calculations for systems with size $N = 4$ can be executed at least to eighth order. Interestingly, fourth order in the magnetic field is not enough to switch between $|0; 1, 1\rangle$ and $|0; -1, 1\rangle$. Up to that order, the result of $\langle 0; 1, 1|0; -1, 1\rangle = -\langle 0; 1, 1| Z_1 |0; 1, 1\rangle$ is identically vanishing. For up to seventh order, it still holds that $\langle 0; 1, 1|0; -1, 1\rangle = 0$, even though there are non-zero terms in this calculation, but they cancel each other out. The eighth order is the first order that suffices to switch between those two states, because

$$\langle 0; 1, 1|0; -1, 1\rangle = \frac{47385}{32}\lambda^8 + \mathcal{O}(\lambda^9).$$

It is not clear why the terms up to this order cancel each other out and it is difficult to investigate, because the number of terms in fourth order is already very big. However, it means that the basis states of our ground-state manifold are to some extend stable with respect to a low magnetic field, even when the system size is $N = 4$.

If we would have taken the CSCO with the loops Z_1 and Z_2 instead, the new basis states of the ground-state manifold would be stable with respect to the magnetic field for all system sizes, because then the perturbation would commute with the loops and cannot be used to switch ground state. But then, the same argument as before holds if we had taken a magnetic field in x-direction.

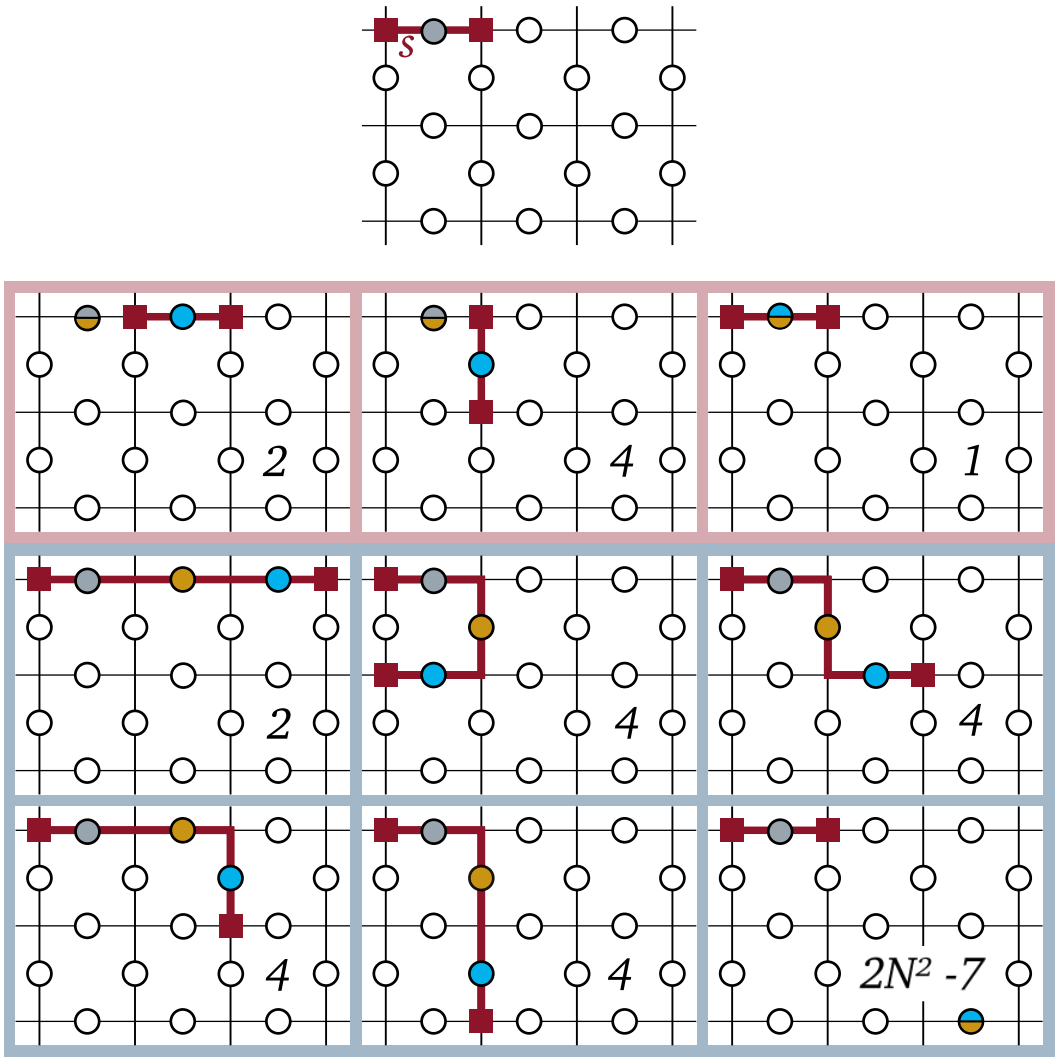

Abbildung 5.2: The upper picture represents the state $|s, s+e_1; 1, 1\rangle = b_s^\dagger b_{s+e_1}^\dagger |0; 1, 1\rangle$. The state $[T_2, T_{-2}] |s, s+e_1; 1, 1\rangle$ is represented in the lower nine pictures. It contains $2N^2 + 18$ summands, namely all possible combinations of non-commuting terms in T_2 and T_{-2}. The pictures with the red background represent the actions of $T_2 T_{-2}$. Their prefactor in the superposition is $+1$. The pictures with the blue background represent the action of $T_{-2} T_2$. Their prefactor is -1. The blue spins represent the action of T_2, the yellow ones the action of T_{-2}. The number in the lower right corner of each picture represents the number of summands represented by that picture. For every picture with the number 2 written on it, the configuration depicted is one of the terms and the other one is obtained by flipping the picture along the vertical line through the grey spin. Analogously, the number 4 represents 4 configurations. One of them is the depicted configuration, the other three are obtained by flipping the picture along the vertical and horizontal line through the grey spin. The picture that represents $2N^2 - 7$ combinations denotes the processes where an excitation is created and then immediately annihilated somewhere in the lattice not in the direct vicinity of the grey spin.

6 Conclusion

We investigated the method of perturbative continuous unitary transformation (pCUT), that can be applied if the unperturbed Hamiltonian has an equidistant spectrum that is bounded from below, such that the Hamiltonian can be expressed in quasi-particle representation. The perturbation Hamiltonian has to consist of operators that create or annihilate a limited number of quasi-particles. Then it is possible to apply a continuous unitary transformation that transformes the perturbed Hamiltonian model-independently to a quasi-particle conserving effective one, in order to diagonalize the separate quasi-particle blocks one after another. All that has been investigated before by Mielke ([5]), Knetter and Uhrig ([6]), and others. We were interested in an explicit expression for the unitary transformation itself, in order to be able to transform other observables or the basis states themselves. The procedure is similar to the derivation of the pCUT formalism and results in a system of recursive differential equations for the coefficients of the unitary transformation. These equations depend also on the coefficient functions used in pCUT which means that the new approach is not faster for problems that only require the effective Hamiltonian. We investigated connections between the coefficient functions used in pCUT, in order to optimize the computer aided implementation, and were able to find a similar connection between the coefficient functions of the unitary transformation. Together with further optimizations, it is possible to calculate this transformation up to at least eleventh order if the perturbation can only create or annihilate two quasi-particles.

In the second part of this thesis we investigated Kitaevs toric code model ([3]). We found a basis in which the Hamiltonian is diagonal and we proved that the ground-state manifold is four-fold degenerate. The toric code perturbed by a low magnetic field is a system for that the pCUT formalism is applicable. We used the effective Hamiltonian to calculate the ground-state energy and to calculate the evolution of a two-particle excitation. We used the effective unitary transformation to calculate that the magnetic field is not able to switch between different basis states of the ground-state manifold.

We have investigated the toric code perturbed by a magnetic field in z-direction. We have discussed that using a magnetic field in x-direction is an analogous case. Vidal, Dusuel and Schmidt have considered in [7] a more general magnetic field with a

component in z-direction and a component in x-direction. Vidal, Thomale, Dusuel and Schmidt have considered in [8] a magnetic field in y-direction. For both results they used the pCUT method described in chapter 2. One possible application for the altered pCUT method from chapter 3 would be to calculate the effective unitary transformation for these systems. Calculating higher orders is not possible as the coefficients of this unitary transformations depend on the coefficients of the effective Hamiltonian, but the transformation could be used to transform the basis states. This would enable us to to calculate for example the topological Rényi entropy of order 2 or Wilson loops as Halász and Hamma did in [9] for the toric code perturbed by a magnetic field in z-direction.

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Declaration

I declare that I have written the thesis by myself and that no sources or aids other than those quoted in the thesis have been used.

Erlangen, 5. April 2019

Lea Lenke