The role of boundaries in one-dimensional gapped phases

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Ich versichere, dass ich die Arbeit selbstständig verfasst und keine anderen als die angegebenen Quellen und Hilfsmittel benutzt sowie Zitate kenntlich gemacht habe.

Madita Franziska Nocon

Aachen, den

Contents

1 Introduction

Phase transitions in general are transitions where a phase, i.e. a state of matter, changes into another state of matter. In classical statistical physics, phase transitions are discontinuous transformations of the whole system as a function of the temperature T. There are so-called first-order phase transitions where the derivative of a thermodynamic potential with respect to the temperature is discontinuous. These phase transitions are the most common as the transitions solid state $\leftrightarrow$ fluid, gas $\leftrightarrow$ fluid, and gas $\leftrightarrow$ solid state are of this type. Aside from these quite ordinary phase transitions, there exist second-order phase transitions where the second derivative of a thermodynamic potential with respect to T is discontinuous. Examples for second-order phase transitions are the transitions ferromagnetic material $\leftrightarrow$ paramagnetic material or superconductor $\leftrightarrow$ non-superconductor.

In contrast, quantum phase transitions occur at absolute zero (what implies that the system is in its ground state), where an external parameter that is not the temperature but e.g. a magnetic field or the pressure causes a discontinuous change in the system's ground states. Due to fluctuations, the system may alter the ground state it is in as a function of this external parameter. Since the system is at zero temperature, there cannot be thermal fluctuations, so these fluctuations belong to the class of quantum fluctuations. This is why corresponding phase transitions are termed quantum phase transitions.

Instead of investigating whether the system is continuous as a function of a specific parameter, it is common to examine how the gap between the ground state energy and the energy of the first excited state behaves. One may imagine this a plausible consequence by considering the variation of the particular parameter as a perturbation and applying perturbation theory: Assuming that there is an energy gap $\Delta > 0$ above the ground state energy, we can approximate the differences of the ground state energy and any other energy of an excited state to be greater than or equal to Δ. The k-th order perturbation theory in the perturbation strength t can then be estimated roughly to be less than or equal to $\frac{|c_k|t^k}{\Delta^{k-1}}$, where $c_k \in \mathbb{R}$ is specific for the k-th order, containing the matrix elements of the perturbation except the perturbation strength. The variation of the energy caused by the perturbation would then be bounded above by $C\Delta \sum_{k=1}^{\infty} \frac{t^k}{\Delta^k}$, where $C := \sup_{k \geq 1} |c_k|$. Choosing the perturbation strength t to be less than the energy gap (what can always be achieved since $\Delta > 0$) implies that the geometric series converges, and therefore the alteration of the energy is continuous and a phase transition cannot happen there.

Aside from this plausibility argument, the characterization that a gap implies a system does not undergo a phase transition can also be proven rigorously using the principle of 'automorphic equivalence'[1]. It defines a phase as an equivalence class, associated with the equivalence relation that two systems are in the same phase if there exists a smooth path of gapped Hamiltonians $H(s)$, $s \in [0, 1]$, where $H(0)$ belongs to one of these phases and $H(1)$ is the Hamiltonian of the other phase[1]. Then their ground states are related by an automorphism that is generated by a quasi-local unitary with almost exponential decay[1]. That means an alteration affecting only one site cannot influence the entire chain and cause a phase transition.

As is turns out, in one dimension, the classification of phases via gap yields different results for open boundary conditions and periodic boundary conditions. Using periodic boundary conditions (such that the system is translation invariant) yields that there is only one phase in one dimension[2, 3].

In contrast, S. Bachmann and B. Nachtergaele introduce a model which is called the product vacua with boundary states (PVBS) of a one-dimensional, gapped quantum spin system with open boundary conditions, and show that these edge states require a finer classification of quantum phases[4]. We are now interested in how these perceptions fit together. Since these investigations are done by using the formalism of matrix product states (MPS), we will also make use of this formalism.

In this thesis, we aim to see whether a vanishing gap also implies a phase transition, i.e. the definitions via gap and discontinuous change in the ground states are equivalent for open boundary conditions. In the case where discontinuities of the ground states occur, we are further interested in the way these discontinuities appear, for example whether the state changes completely or only at the boundary if we add a perturbation that acts on the boundary only.

The PVBS-model that we will examine describes gapped phases, i.e. the energy of the first excited state is always bounded below by a positive constant, even in the thermodynamic limit[2]. So we have to modify the Hamiltonian in order to force the gap to close. As it will turn out, we just have to do that at the boundary.

The model under consideration has the specific property that the corresponding Hamiltonian depends on certain parameters which determine how strong particles bind to the boundaries. Thus, we can construct a simple path on which the gap vanishes.

We will especially analyze the behavior of the ground states if various perturbations are taken into the Hamiltonian. As we will see, depending on the Hilbert space dimension and the perturbation, the examination is more or less complicated. We also will find more than one way to construct a path on which the gap closes.

Another point of interest is whether we can obtain a Hamiltonian that is completely translation invariant and therefore equal to the one with periodic boundary conditions. This will prove an aim that can be achieved in some cases more or less to our satisfaction.

As we will ascertain, a vanishing gap causes the ground state degeneracy to alter, but this fact will not have an effect on the entire chain as the only change happens at the boundary. Thus, we may not call this a phase transition since the bulk state does not undergo any changes at all.

In addition, we investigate the long-distance description of this system by applying Renormalization Group transformations. As these results are not entirely satisfying due to a certain instability, we develop a modified form of PVBS that is capable of avoiding these inconveniences. These new PVBS are subsequently examined and we will see that this modified form of PVBS also eliminates the difficulties that we encounter while examining phase transitions.

2 Matrix Product States

Consider a system of N subsystems, for example N particles that can attain r states. Then, an arbitrary wave function describing the total system is given by

$$|\Psi\rangle = \sum_{i_1,i_2,\ldots,i_N=1}^{r} c_{i_1,i_2,\ldots,i_N} |i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_N\rangle =: \sum_{i_1,i_2,\ldots,i_N=1}^{r} c_{i_1,i_2,\ldots,i_N} |i_1 i_2 \cdots i_N\rangle, \tag{2.1}$$

where $c_{i_1,i_2,\ldots,i_N} \in \mathbb{C}$, $i_1,\ldots,i_N = 1,2,\ldots,r$, and $\{|1\rangle,|2\rangle,\ldots,|r\rangle\}$ is a basis of the subsystem.

The number of the constants $c_{i_1,\ldots,i_N}$ increases exponentially with N, as does the Hilbert space, but not all possible states in the Hilbert space are equally appropriate as ground states[5]. As there are usually nearest and next-to-nearest neighbor interactions in nature, and low-energy eigenstates of local, gapped Hamiltonians follow the area-law for the entanglement entropy, most of the states contained in the Hilbert space are not suitable as ground states[5]. The area-law of entanglement entropy states that the entropy of a subsystem scales with the size of the boundary of this subsystem. Fortunately, for most states of the Hilbert space, the entropy of the system scales with the volume instead of the boundary, and therefore the relevant part of the Hilbert space is, in comparison, extremely small[5]. In one dimension, an efficient notation for these relevant states is given by matrix product states (MPS)[5].

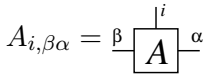
Written as a MPS with open boundary conditions, $|\Psi\rangle$ is given by[6]:

$$|\Psi\rangle = \sum_{i_1,i_2,\ldots,i_N=1}^{r} A^{(1)}_{i_1} A^{(2)}_{i_2} \cdots A^{(N)}_{i_N} |i_1 i_2 \cdots i_N\rangle, \tag{2.2}$$

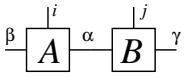
where $A^{(1)}_{i_1} \in \mathrm{Mat}(\mathbb{C})^{1\times D}$, $A^{(2)}_{i_2},\ldots,A^{(N-1)}_{i_{N-1}} \in \mathrm{Mat}(\mathbb{C})^{D\times D}$ and $A^{(N)}_{i_N} \in \mathrm{Mat}(\mathbb{C})^{D\times 1}$, $i_1,i_2,\ldots,i_N = 1,2,\ldots,r$. In the case of periodic boundary conditions, $|\Psi\rangle$ can be written as

$$|\Psi\rangle = \sum_{i_1,i_2,\ldots,i_N=1}^{r} \mathrm{Tr}\left(A^{(1)}_{i_1} A^{(2)}_{i_2} \cdots A^{(N)}_{i_N}\right) |i_1 i_2 \cdots i_N\rangle, \tag{2.3}$$

where $A^{(1)}_{i_1},\ldots,A^{(N)}_{i_N} \in \mathrm{Mat}(\mathbb{C})^{D\times D}$[6]. The matrices $A^{(k)}_{i_k}, k = 1,\ldots,N$, $i_k = 1,\ldots,r$ can be understood as three-index tensors and represented in a graphical language as[6]

$$A_{i,\beta\alpha} = \beta \text{ — } \boxed{A} \text{ — } \alpha \quad , \tag{2.4}$$


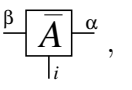
where i is the physical index, i.e. the index that indicates the physical state. The connection between two such diagrams



means summing over the index α[6]:

$$\sum_{i=1}^{D} A_{i,\beta\alpha} B_{j,\alpha\gamma} \tag{2.5}$$

The complex conjugate of a matrix is represented by



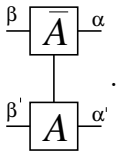
where the physical index is directed downwards.

2.1 Transfer Matrices

The transfer matrix is defined as

$$T = \sum_{i=1}^{r} A_i \otimes \bar{A}_i, \tag{2.6}$$

and determines a MPS up to a local unitary transformation: if $\sum_{i=1}^{r} A_i \otimes \bar{A}_i = \sum_{i=1}^{r} B_i \otimes \bar{B}_i$, then $A_i = \sum_{j=1}^{r} v_{ij} B_j$, where (v_{ij}) is an isometry[6]. In the graphical language, the transfer matrix is depicted as

$T =$ 

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2.1.1 An Application to Renormalization Group Transformations

In order to obtain the long-distance information of a system, we can use a Renormalization Group (RG) technique. The short-distance information is integrated out and length and operators are rescaled, restoring the initial form[7]. In the case of a one-dimensional system with N subsystems of r-dimensional Hilbert spaces, two neighboring subsystems are joined to a new subsystem, and operators and length are rescaled[7]. Then, states equal up to a local unitary operation have to be identified[7]. This transformation can be executed by using the transfer matrix (2.6), which is invariant under local unitary operations[7]. The RG transformation corresponds to $T \mapsto T' = T^2$[7].

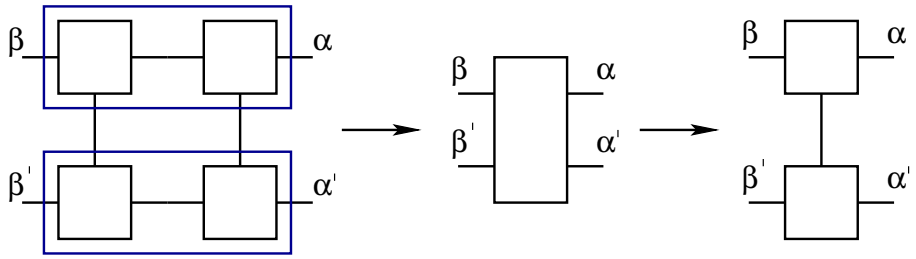

Figure 2.1: The figure depicts the RG transformation of the transfer matrix expressed in the graphical language.

The process is shown in Fig. 2.1 in the graphical language. Squaring the transfer matrix means we can interpret two multiplied matrices as a new one with two physical indices which are summed over. The four left, free indices can now be understood as those of a four-index tensor, depicted in the middle of the figure. This tensor can then be written as a sum of tensor products of matrices with their complex conjugates. The number r' of terms in the sum (i.e. the required number of matrices) is between r and r^2. The physical meaning of this is that, in the case $r' = r$, the number of possibilities of the combined states is equal to the former number of states; and if $r' > r$, additional possibilities arise. The fact that $r' \leq r^2$ is also reasonable as there cannot be more possibilities than the number of 2-combinations of the set of states, i.e. the order is irrelevant. As it turns out, r' can be calculated by computing the Kraus rank of T^2: Although T^2 is a tensor with four indices $T^2_{\beta'\beta\alpha'\alpha}$, we can interpret it as a matrix $T^2_{(\beta'\beta)(\alpha'\alpha)}$. Rearranging the matrix elements yields a new matrix $K_{(\beta'\alpha')(\beta\alpha)}$. The rank of K is the Kraus rank of T^2 and corresponds to r'.

By applying the transformation p times and then taking the limit $p \to \infty$, only the long distance information is preserved.

2.2 Construction of the Parent Hamiltonian

Given a set of desired ground states

$$|\Psi(B)\rangle = \sum_{i_1,\ldots,i_N=1}^{r} \mathrm{Tr}(BA_{i_1}\cdots A_{i_N})|i_1\ldots i_N\rangle, \tag{2.7}$$

where $B, A_{i_1}, \ldots, A_{i_N} \in \mathrm{Mat}(\mathbb{C})^{D\times D}$, and B describes some boundary conditions, we want to construct the parent Hamiltonian, i.e. the Hamiltonian with its ground states given by $|\Psi(B)\rangle$. We would like the parent Hamiltonian H to be frustration free, i.e. $H = \sum_{k=1}^{N-1} h_{k,k+1}$, where $h_{k,k+1} \geq 0$ acts on sites k and $k+1$ and already minimizes the energy on these two sites of the global ground state[8]. Therefore, we concentrate on the sites k and $k+1$ and fix $i_1, \ldots, i_{k-1}, i_{k+2}, \ldots, i_N \in \{1, 2, \ldots, r\}$. Then, $|\Psi(B)\rangle$ for fixed $i_1, \ldots i_{k-1}, i_{k+2}, \ldots, i_N$ can be recast in the reduced space as

$$\begin{aligned}
|\Psi(B, i_1, \ldots i_{k-1}, i_{k+2}, \ldots, i_N)\rangle &:= \sum_{i_k,i_{k+1}=1}^{r} \mathrm{Tr}(BA_{i_1}\cdots A_{i_k}A_{i_{k+1}}\cdots A_{i_N})|i_k i_{k+1}\rangle && (2.8)\\
&= \sum_{i_k,i_{k+1}=1}^{r} \mathrm{Tr}(\underbrace{A_{i_{k+2}}\cdots A_{i_N}BA_{i_1}\cdots A_{i_{k-1}}}_{=:B_{i_1\ldots i_{k-1}i_{k+2}\ldots i_N}} A_{i_k}A_{i_{k+1}})|i_k i_{k+1}\rangle && (2.9)\\
&= \sum_{i_k,i_{k+1}=1}^{r} \mathrm{Tr}(B_{i_1\ldots i_{k-1}i_{k+2}\ldots i_N}A_{i_k}A_{i_{k+1}})|i_k i_{k+1}\rangle. && (2.10)
\end{aligned}$$

In order for $|\Psi(B, i_1, \ldots i_{k-1}, i_{k+2}\ldots i_N)\rangle$ to be the ground states of $h_{k,k+1}$, we define

$$h_{k,k+1} = \Pi_{\Psi_k\perp} = \mathbb{1} - \Pi_{\Psi_k}, \tag{2.11}$$

where $\Pi_{\Psi_k\perp}$ denotes the projector onto an orthogonal complement of

$$\mathrm{span}\{\, |\Psi(B, i_1, \ldots, i_{k-1}, i_{k+2}, \ldots, i_N)\rangle \,|\, B \in \mathrm{Mat}(\mathbb{C})^{D\times D}\} =: \mathcal{G} \tag{2.12}$$

and Π_{Ψ_k} denotes the projector onto the subspace $\mathcal{G}$.

Since $h_{k,k+1}$ ($k = 1, \ldots, N-1$) are projectors, all eigenvalues of $h_{k,k+1}$ and H are non-negative, and as $\mathcal{G}$ is the eigenspace of $h_{k,k+1}$ corresponding to the eigenvalue zero, it is also the eigenspace of H corresponding to the eigenvalue zero and hence the ground state space:

$$\begin{aligned}
H|\Psi(B)\rangle &= \sum_{k=1}^{N-1} h_{k,k+1}|\Psi(B)\rangle && (2.13)\\
&= \sum_{k=1}^{N-1}\sum_{i_1,\ldots,i_N=1}^{r} h_{k,k+1}\mathrm{Tr}(BA_{i_1}\cdots A_{i_N})|i_1\ldots i_N\rangle && (2.14)\\
&= \sum_{k=1}^{N-1}\sum_{\substack{i_1,\ldots,i_{k-1},\\ i_{k+2},\ldots,i_N=1}}^{r} |i_1\ldots i_{k-1}\rangle \otimes \Big(\underbrace{h_{k,k+1}|\Psi(B, i_1, \ldots, i_{k-1}, i_{k+2}, \ldots, i_N)\rangle}_{=0}\Big) \otimes |i_{k+2}\ldots i_N\rangle && (2.15)\\
&= 0, && (2.16)
\end{aligned}$$

where we used Eq. (2.7) and (2.8).

3 Product Vacua with Boundary States

A special type of MPS are the Product Vacua with Boundary States (PVBS) introduced by S. Bachmann and B. Nachtergaele[4]. As this model forms the primary subject of our studies, we give a brief review on its properties.

Considering a quantum spin chain of length L with nearest-neighbor interaction, the ground state degeneracy is 2^n, where n can be interpreted as the number of distinguishable particles added to the product vacuum. An arbitrary product state is given by $|i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_L\rangle =: |i_1 i_2 \dots i_L\rangle$, where $i_1, \dots, i_L = 0, 1, \dots, n$. The number of different values which $i_1, \dots, i_L$ can attain is called the dimension d of the Hilbert space. The integers $1, \dots, n$ label the particles and 0 represents the vacuum. The matrices $v_0, v_1, \dots, v_n \in \mathrm{Mat}(\mathbb{C})^{2^n \times 2^n}$ generating the ground states satisfy the commutation relations

$$v_i v_j = e^{i\vartheta_{ij}} \lambda_i \lambda_j^{-1} v_j v_i, \qquad i \neq j \tag{3.1}$$

$$v_i^2 = 0, \qquad i \neq 0 \tag{3.2}$$

where ϑ_{ij} and $0 \neq \lambda_i$ are real numbers, and $\vartheta_{ij} = -\vartheta_{ji}$ for $0 \leq i, j \leq n$[4]. λ_i can be chosen to be positive by redefining the phases ϑ_{ij}, and we set $\lambda_0 = 1$ for normalization purposes[4]. To prove the existence of such matrices, S. Bachmann and B. Nachtergaele give an example[4]:

$$v_0 = \bigotimes_{i=1}^{n} P_{0i}^2 w_i \tag{3.3}$$

$$v_i = \bigotimes_{j=1}^{i-1} P_{ij} w_j \otimes \sigma^+ \otimes \bigotimes_{k=i+1}^{n} P_{ik} w_k, \qquad i = 1, \dots, n \tag{3.4}$$

where

$$\sigma^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad w_i = \begin{pmatrix} 1 & 0 \\ 0 & \lambda_i \end{pmatrix}, \quad P_{ij} = \begin{pmatrix} e^{\frac{1}{2} i\vartheta_{ij}} & 0 \\ 0 & 1 \end{pmatrix}. \tag{3.5}$$

The matrices v_i constructed in this way satisfy the commutation relations (Eq. (3.1) and (3.2)), and generate the MPS

$$\psi(B) = \sum_{i_1, \dots, i_L = 0}^{n} \mathrm{Tr}(B v_{i_L} \dots v_{i_1}) |i_1 \dots i_L\rangle, \tag{3.6}$$

where $B \in \mathrm{Mat}(\mathbb{C})^{2^n \times 2^n}$. Due to the commutation relation (3.1), a particle of type i, $i = 1, 2, \dots, d-1$, binds to the left edge if $\lambda_i < 1$, to the right edge if $\lambda_i > 1$, or to neither edge in the case $\lambda_i = 1$. These states never contain two particles of the same type on the chain because applying Eq. (3.1) enables transpositions of v_i and v_j until two v_i are next to each other and then by making use of Eq. (3.2) the trace vanishes.

In order to construct the parent Hamiltonian with ground states $\psi(B)$ of a chain with arbitrary length L, we first only need to concentrate on a chain of length $L = 2$, as seen in section 2.2. In the case $L = 2$, the vectors

$$\phi_i = |0i\rangle - e^{-i\vartheta_{i0}} \lambda_i |i0\rangle \tag{3.7}$$

$$\phi_{ij} = |ij\rangle - e^{-i\vartheta_{ji}} \lambda_i^{-1} \lambda_j |ji\rangle \tag{3.8}$$

$$\phi_{ii} = |ii\rangle, \tag{3.9}$$

for $1 \leq i, j \leq n$ and $i \neq j$ are orthogonal to the MPS $\psi(B)$, $\forall B$. Therefore, for $L = 2$, the states $\{\psi(B) \,|\, B \in \mathrm{Mat}(\mathbb{C})^{2^n \times 2^n}\}$ are eigenstates of the Hamiltonian

$$h = \sum_{i=1}^{n} |\hat{\phi}_i\rangle\langle\hat{\phi}_i| + \sum_{1 \leq i \leq j \leq n} |\hat{\phi}_{ij}\rangle\langle\hat{\phi}_{ij}|, \tag{3.10}$$

where $\hat{\cdot}$ indicates normalization. The parent Hamiltonian for a chain of length $L > 2$ is then given by

$$H = \sum_{x=1}^{L-1} h_{x,x+1}, \tag{3.11}$$

where

$$h_{x,x+1} = \underbrace{\mathbb{1} \otimes \cdots \otimes \mathbb{1}}_{x-1 \text{ times}} \otimes h \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1} \tag{3.12}$$

represents a nearest-neighbor interaction. By construction, H is the parent Hamiltonian of the ground states $\psi(B)$ mentioned in Eq. (3.6)[4].

The case $\lambda_i = 1$, for any arbitrary $i \in \{1, 2, \ldots, d-1\}$, is a special case since the particle of type i binds neither to the left nor the right edge. Moreover, the statement that the energy of the first excited state is always bounded below by a positive constant[4] only holds for $\lambda_i \neq 1$, $\forall i \in \{1, 2, \ldots, d-1\}$. Fig. 3.1 illustrates the energy of the first excited state of H for $n = 1$ and $L = 2, 3, \ldots 20$. As the energy decreases strictly monotonically as a function of L, the gap may close in the limit $\lambda \to \infty$. Bachmann and Nachtergaele actually show that the gap closes in the thermodynamic limit whenever there is $\lambda_i = 1$ for any $i \in \{1, 2, \ldots, d-1\}$[9].

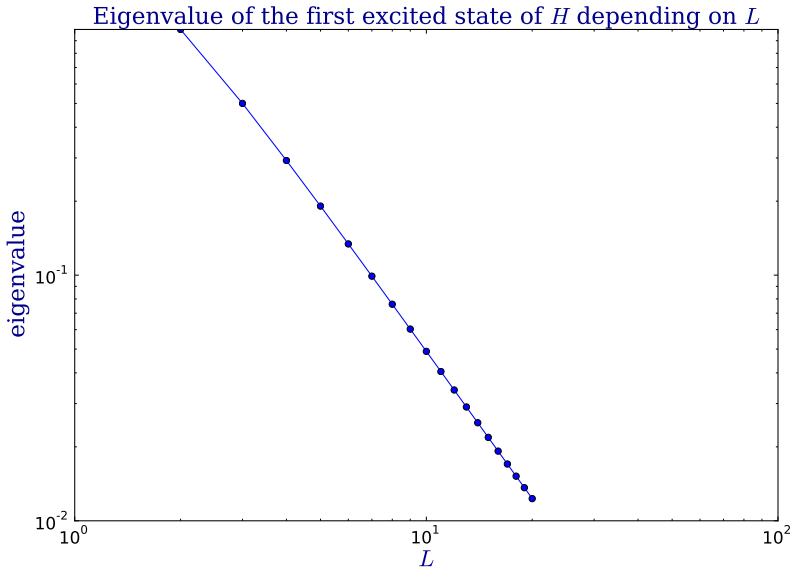

Figure 3.1: The plot visualizes the dependence of the eigenvalue of the first excited state of H for $\lambda = 1$ on L. The axes-scaling is log-log. For large L, the numerical result for the slope is approximately 2. Therefore, the eigenvalue decreases $\sim \frac{1}{L^2}$.

Although PVBS are only defined for open boundary conditions, we are further interested in what happens when using periodic boundary conditions. For this, we set $B = \mathbb{1}$ what has the same effect as no B at all. Since then all v_i with $i \neq 0$ are traceless because they contain σ^+ (cf. Eq. (3.5)), the only remaining ground state is $|0 \dots 0\rangle$. Therefore, PVBS with periodic boundary conditions have always, independently of n and L, a non-degenerate ground state.

In the next chapter, we will have a closer look at the case of open boundary conditions and analyze whether phase transitions are possible in this case.

4 Phase Transitions

In this chapter, we strive to examine whether a vanishing gap implies a phase transition for the PVBS-model in the case of open boundary conditions. We will analyze paths on which n changes for the cases $d = 2$ (one particle type) and $d = 3$ (two particle types). For this purpose, we first take the limits $\lambda_i \to 0$, $i = 1, \ldots, d-1$, to obtain a path as simple as possible for a change in the number n of particle types occurring in the ground states. Physically, the limit $\lambda_i \to 0$ means that a particle of type i extremely binds to the left edge.

Since the commutation relation (3.1) does not hold in the limit $\lambda_i \to 0$, there may occur discontinuities. So we investigate the ground states in the limit in two ways and see whether they yield the same results. One way is to look at the Hamiltonian as a function of λ_i, and calculate its ground states; and in the other way, we start with the ground states from Eq. (3.6). First we apply the commutation relations (3.1) and (3.2), and then we take the limits $\lambda_i \to 0$. Subsequently, we examine whether the ground states are equal, and we also check the numerical result for discontinuities. For this purpose, we wrote a program that calculates the Hamiltonian and determines its eigenvalues dependent on the parameters λ_i and various perturbation strengths. Once we ascertained that the limits are continuous and the ground states of both analyzed ways are consistent, we add perturbations that act on the boundary and investigate what happens to the ground states and the Hamiltonian.

We aim to change n while the dimension d of the Hilbert space remains constant. But the PVBS-model introduced by S. Bachmann and B. Nachtergaele in [4] only considers the cases $n = d - 1$; so how do we understand the case where $n < d - 1$? Since d is the dimension of the Hilbert space and constant, it still provides $d - 1$ various particle types or the vacuum to be on a site. But not all of these possibilities occur in the ground states; only $n < d - 1$ particle types or the vacuum are possible site occupancies.

If $n = 0$, we only expect the product vacuum $|0 \ldots 0\rangle$ to be a valid ground state. Therefore, we want the Hamiltonian to be of the form

$$H = \sum_{k=1}^{d-1} \sum_{i=1}^{L} |k\rangle\langle k|_i, \tag{4.1}$$

because then, every particle type on every site gains an energy > 0 and would not belong to the ground state space. Moreover, this Hamiltonian is completely translation invariant, and therefore equivalent to the one with periodic boundary conditions.

For any other $0 < n < d-1$, the sum $\sum_{i=1}^{L}$ in Eq. (4.1) has to be replaced by $\sum_{i=2}^{L}$ for those k still occurring in the ground states.

As we will see, in the case of dimension $d = 2$, the transition of n from 1 to 0 yields the Hamiltonian that we expect to obtain for the case $n = 0$, $d > 1$. In the case $d = 3$, there will be more difficulties and the Hamiltonian we find will still contain terms of a two-particle interaction. Nevertheless, we will be able to change n and with it the ground state degeneracy, but this will only have an effect on the boundary.

4.1 One Particle Type: The Case $d = 2$

Let us consider the case $n = 1$, and see whether n can be changed to $n = 0$ only by manipulating the Hamiltonian at the boundary, and investigate what happens to the state.

First, we examine the ground states by taking the limit $\lambda \to 0$ of the Hamiltonian. For that, we look at the Hamiltonian acting on two neighboring sites that is, according to Eq. (3.10), given by

$$\begin{aligned} h &= |\hat{\phi}_1\rangle\langle\hat{\phi}_1| + |\hat{\phi}_{11}\rangle\langle\hat{\phi}_{11}| \\ &= \frac{1}{1+\lambda^2}\left(|01\rangle - e^{-i\vartheta_{10}}\lambda|10\rangle\right)\left(\langle 01| - e^{i\vartheta_{10}}\lambda\langle 10|\right) + |11\rangle\langle 11| \end{aligned}$$

where $\lambda \neq 0$ and ϑ_{10} are arbitrary real numbers. For $\lambda \to 0$, this Hamiltonian can be written as:

$$\lim_{\lambda\to 0} h = |01\rangle\langle 01| + |11\rangle\langle 11| = \mathbb{1} \otimes |1\rangle\langle 1| \tag{4.2}$$

In order to indicate that h acts on sites x and $x+1$, we write $h_{x,x+1}$. In the case of vanishing λ, the commutator $[h_{x,x+1}, h_{y,y+1}]$, where $x, y = 1, 2, \ldots L-1$, also vanishes since the operators are diagonal. For that reason, the eigenvalues of the Hamiltonian on the entire chain

$$H = \sum_{i=1}^{L-1} h_{i,i+1} = \sum_{i=1}^{L-1} |1\rangle\langle 1|_{i+1}, \tag{4.3}$$

where $(\,\cdot\,)_{i+1}$ denotes that $\cdot$ acts on site $i+1$, are all integers and actually ≥ 0 since H is a projector. Accordingly, vectors with eigenvalue zero must be ground states. Fig 4.1 shows the dependence of the eigenvalues on λ, and for $\lambda \to 0$, the eigenvalues become non-negative integers. The curves are continuous in the limit as well.

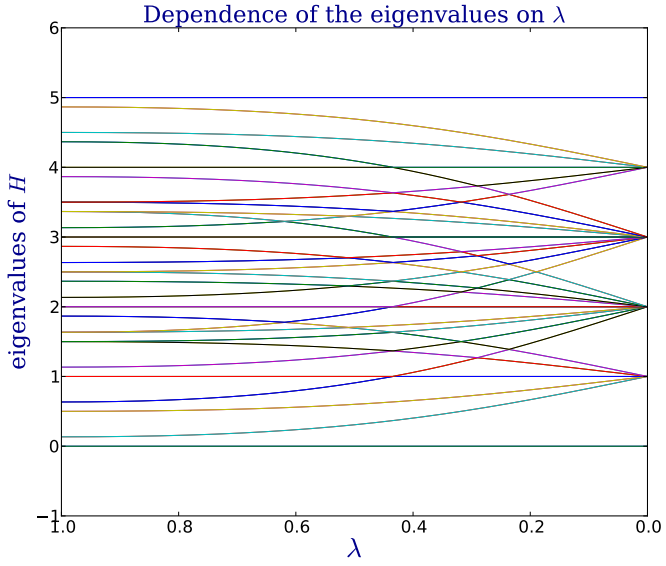

Figure 4.1: The plot of the dependence of the eigenvalues of $H = \sum_{i=1}^{L-1}\left(\left(\frac{1}{1+\lambda^2}\left(|01\rangle - e^{-i\vartheta_{10}}\lambda|10\rangle\right)\left(\langle 01| - e^{i\vartheta_{10}}\lambda\langle 10|\right)\right)_{i,i+1} + |11\rangle\langle 11|_{i,i+1}\right)$ on λ is exemplarily shown for a chain of length $L = 6$. For larger L, there are more curves, even for higher eigenvalues, but they behave quite the same. As $\lambda \to 0$, the curves are continuous and for $\lambda = 0$ the eigenvalues are non-negative integers.

Now, let us see what the ground states of the Hamiltonian in the case $\lambda \to 0$ are. The only vectors that correspond to a zero eigenvalue are

$$|\psi^0\rangle := |0 \dots 0\rangle \tag{4.4}$$

and

$$|\psi^1\rangle := |10 \dots 0\rangle \tag{4.5}$$

since every vector containing a particle on any site but the first one has at least eigenvalue 1. Therefore, (4.4) and (4.5) are the only ground states we obtain in this way.

Now, we apply the second way of calculating the ground states in the limit $\lambda \to 0$, where we start with the ground states $\psi(B)$. As mentioned previously, the commutation relation (3.1) does not hold in the limit $\lambda \to 0$ because $v_1 v_0 \to 0$ for $\lambda \to 0$, but $\lim_{\lambda \to 0} v_0 v_1 \neq 0$. Thus, we have to apply the commutation relations (3.1) and (3.2) before taking the limit in order to obtain the right ground states. So starting with $\psi(B)$ defined in Eq. (3.6) and using the commutation relations (3.1) and (3.2) leads to

$$\begin{aligned}\psi(B) &= \mathrm{Tr}(Bv_0 \dots v_0)|0 \dots 0\rangle + \mathrm{Tr}(Bv_0 \dots v_0 v_1)|10 \dots 0\rangle + \dots + \mathrm{Tr}(B \underbrace{v_1 v_0}_{e^{i\vartheta_{10}}\lambda_1 v_0 v_1} \dots v_0)|0 \dots 01\rangle \\ &= \mathrm{Tr}(Bv_0 \dots v_0)|0 \dots 0\rangle \\ &+ \mathrm{Tr}(Bv_0 \dots v_0 v_1)\left(|10 \dots 0\rangle + e^{i\vartheta_{10}}\lambda_1 |010 \dots 0\rangle + \dots + \left(e^{i\vartheta_{10}}\lambda_1\right)^{L-1}|0 \dots 01\rangle\right). \end{aligned} \tag{4.6}$$

Taking the limit of Eq. (4.6), we obtain

$$\lim_{\lambda \to 0} \psi(B) = \mathrm{Tr}(Bv_0 \dots v_0)|0 \dots 0\rangle + \mathrm{Tr}(Bv_0 \dots v_0 v_1)|10 \dots 0\rangle \tag{4.7}$$

which can either span a two-dimensional space or only a one-dimensional space what would happen if $\mathrm{Tr}(Bv_0 \dots v_0)$ and $\mathrm{Tr}(Bv_0 \dots v_0 v_1)$ depend on the same matrix elements of B, and could therefore not be chosen independently. Fortunately, the ground states consistently span the same space as (4.4) and (4.5), as can be seen by the matrices v_i, constructed in Eq. (3.3) and (3.4) and the following choice of B:

$$v_0 = \begin{pmatrix} e^{i\vartheta_{01}} & 0 \\ 0 & \lambda_1 \end{pmatrix}, \quad v_1 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} c_1 & 0 \\ c_2 & 0 \end{pmatrix},$$

where $c_1, c_2 \in \mathbb{C}$. Then, the traces are

$$\mathrm{Tr}(Bv_0 \dots v_0) = c_1 e^{iL\vartheta_{01}}, \qquad \mathrm{Tr}(Bv_0 \dots v_0 v_1) = c_2 e^{i(L-1)\vartheta_{01}}.$$

Since c_1 and c_2 are arbitrary complex numbers and therefore every arbitrary linear combination can be constructed, the ground state space is two-dimensional. These states represent the empty chain ($|0 \dots 0\rangle$), and the chain with one particle sticking to the left edge ($|10 \dots 0\rangle$).

Let us now investigate whether the system undergoes a phase transition if we add a perturbation of the form

$$S = \gamma |1\rangle\langle 1| \otimes \mathbb{1}_{L-1} = \gamma |1\rangle\langle 1|_1, \qquad \gamma > 0, \tag{4.8}$$

where $\mathbb{1}_{L-1}$ denotes the identity map acting on $L-1$ sites, and γ denotes the perturbation strength. This perturbation might be caused by e.g. a local magnetic field. When added to the Hamiltonian H, it removes the degeneracy of the ground state. Since H commutes with S,

and both are self-adjoint, there exists a common eigenbasis (fortunately, this eigenbasis is the product basis) and the new eigenvalues can be obtained by the sum of the eigenvalues of H and S. As a result, the former ground state $|10\dots0\rangle$ now corresponds to the energy γ, so $|0\dots0\rangle$ is the only remaining ground state. The elimination of the degeneracy can also be seen in Fig. (4.2) as the ground state energy splits into two energies. If $\gamma \to 1$, the Hamiltonian $H' := H + S$ can be written as

$$H' = \sum_{i=1}^{L} |1\rangle\langle 1|_i, \tag{4.9}$$

which implies that all the sites are equivalent as in the case of periodic boundary conditions. This is the desired form for a Hamiltonian with $n = 0$ mentioned in Eq. (4.1). Since the ground state energy is not degenerate, but the Hilbert space still supports a particle, even though it appears only in excited states, the Hamiltonian H' belongs to the case $n = 0$ and $d = 2$. Thus, we were able to achieve an alteration of the ground state degeneracy only by modifying the boundary, but the change of the ground state space just has an effect at the edge. So the bulk of the system behaves continuously, and therefore this behavior should not fall in the definition of a phase transition.

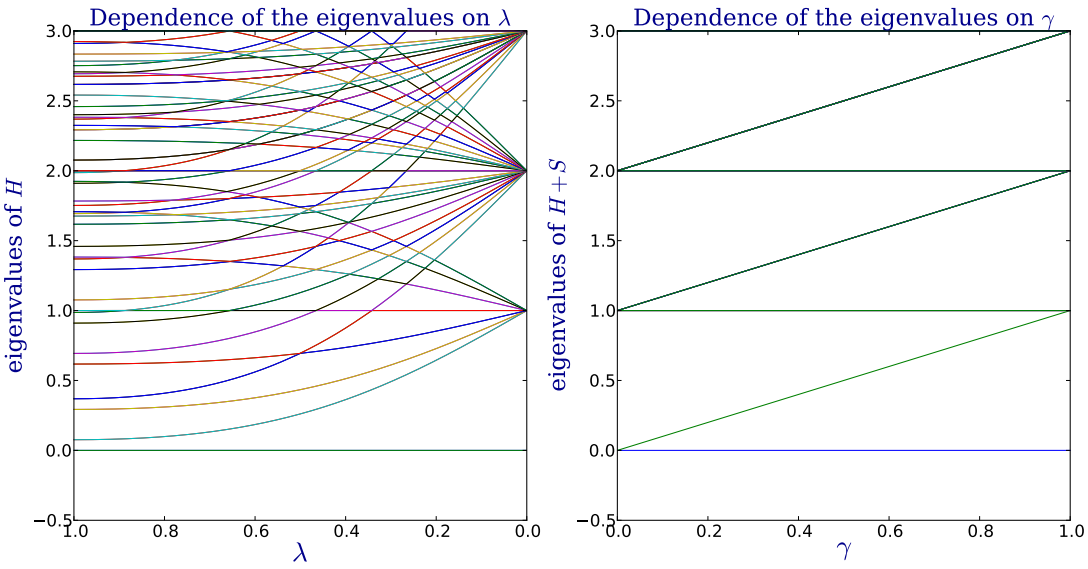

Figure 4.2: On the left, the limit $\lambda \to 0$ for $L = 4$ is shown again in order to indicate the behavior of the eigenvalues. The plot does not show the full spectrum since we are interested in the low-energy states. On the right, the dependence of the eigenvalues of $H + S = \sum_{i=2}^{L} |1\rangle\langle 1|_i + \gamma|1\rangle\langle 1|_1$ on γ for $\gamma \in [0, 1]$ and $L = 4$ is depicted. Some degeneracies are removed for non-vanishing γ as the eigenvalues split up; some of them increase linearly with γ and others remain constant. For excited states, the degeneracies are not completely removed as we see more than two curves intersect at the integers in the plot on the left, but only two split up in the right plot. However, for $\lambda = 0$ and $\gamma = 0$, the ground states are $|0\dots0\rangle$ and $|10\dots0\rangle$, and for $\gamma > 0$ they split up; thus the ground state is not degenerate for $\gamma > 0$. The linear increase underlines the fact that the Hamiltonian H and the perturbation S have a common eigenbasis.

4.2 Two Particle Types: The Case $d = 3$

The next case for which we investigate the system's behavior if the gap closes is the case $n = 2$ and $d = 3$. The Hamiltonian acting on two neighboring sites is created by applying Eq. (3.10) and reads

$$\begin{aligned} h &= |\hat{\phi}_1\rangle\langle\hat{\phi}_1| + |\hat{\phi}_2\rangle\langle\hat{\phi}_2| + |\hat{\phi}_{11}\rangle\langle\hat{\phi}_{11}| + |\hat{\phi}_{12}\rangle\langle\hat{\phi}_{12}| + |\hat{\phi}_{22}\rangle\langle\hat{\phi}_{22}| \\ &= \frac{1}{1+\lambda_1^2}\left(|01\rangle - e^{-i\vartheta_{10}}\lambda_1|10\rangle\right)\left(\langle 01| - e^{i\vartheta_{10}}\lambda_1\langle 10|\right) + |11\rangle\langle 11| \\ &+ \frac{1}{1+\lambda_2^2}\left(|02\rangle - e^{-i\vartheta_{20}}\lambda_2|20\rangle\right)\left(\langle 02| - e^{i\vartheta_{20}}\lambda_2\langle 20|\right) + |22\rangle\langle 22| \\ &+ \frac{1}{\lambda_1^2+\lambda_2^2}\left(\lambda_1|12\rangle - e^{-i\vartheta_{21}}\lambda_2|21\rangle\right)\left(\lambda_1\langle 12| - e^{i\vartheta_{21}}\lambda_2\langle 21|\right), \end{aligned}$$

where $\lambda_1, \lambda_2 \in \mathbb{R}_{>0}$ and $\vartheta_{10}, \vartheta_{20}, \vartheta_{21} \in \mathbb{R}$.

As there are two λs, we have more possibilities for taking the limit $\lambda_1 \to 0$ and $\lambda_2 \to 0$ than in the case $d = 2$. First we study the limit $\lambda_1 \to 0$, $\lambda_2 \to 0$ with constant ratio $\frac{\lambda_1}{\lambda_2} =: \alpha$. Subsequently we examine what happens when taking the limit $\lambda_1 \to 0$ before the limit $\lambda_2 \to 0$.

4.2.1 Constant Ratio α

Starting with the case $\alpha = \frac{\lambda_1}{\lambda_2} = \text{const.}$, we obtain for the Hamiltonian acting on two adjacent sites

$$\begin{aligned} \lim_{\substack{\lambda_1\to 0\\ \lambda_2\to 0, \frac{\lambda_1}{\lambda_2}=\alpha}} h &= |01\rangle\langle 01| + |02\rangle\langle 02| + |11\rangle\langle 11| + |22\rangle\langle 22| \qquad (4.10) \\ &+ \frac{1}{\alpha^2+1}\left(\alpha|12\rangle - e^{-i\vartheta_{21}}|21\rangle\right)\left(\alpha\langle 12| - e^{i\vartheta_{21}}\langle 21|\right) \\ &= \mathbb{1}\otimes|1\rangle\langle 1| + \mathbb{1}\otimes|2\rangle\langle 2| - \frac{1}{\alpha^2+1}\left(|12\rangle + e^{-i\vartheta_{21}}\alpha|21\rangle\right)\left(\langle 12| + e^{i\vartheta_{21}}\alpha\langle 21|\right). \qquad (4.11) \end{aligned}$$

So in this limit, the Hamiltonian of the entire chain is given by

$$\begin{aligned} H &= \sum_{i=1}^{L-1} h_{i,i+1} \qquad (4.12) \\ &= \sum_{i=2}^{L}|1\rangle\langle 1|_i + \sum_{i=2}^{L}|2\rangle\langle 2|_i - \frac{1}{\alpha^2+1}\sum_{i=1}^{L-1}\left(\left(|12\rangle + e^{-i\vartheta_{21}}\alpha|21\rangle\right)\left(\langle 12| + e^{i\vartheta_{21}}\alpha\langle 21|\right)\right)_{i,i+1}, \qquad (4.13) \end{aligned}$$

where $h_{i,i+1}$ is defined as in Eq. (3.12).

To investigate the ground states of this Hamiltonian, we start with investigating the eigenstates of h. In the product basis, h is almost diagonal. The only subspace h is not diagonal in is the space spanned by $|12\rangle$ and $|21\rangle$. Diagonalizing the matrix

$$\begin{pmatrix} \frac{1}{1+\alpha^{-2}} & \frac{-e^{i\vartheta_{21}}\alpha^{-1}}{1+\alpha^{-2}} \\ \frac{-e^{-i\vartheta_{21}}\alpha^{-1}}{1+\alpha^{-2}} & \frac{\alpha^{-2}}{1+\alpha^{-2}} \end{pmatrix}$$

yields the additional eigenstates $\frac{|12\rangle+e^{-i\vartheta_{21}}\alpha|21\rangle}{\sqrt{1+\alpha^2}}$ and $\frac{|12\rangle-e^{-i\vartheta_{21}}\alpha^{-1}|21\rangle}{\sqrt{1+\alpha^{-2}}}$. The eigenstates that belong to zero energy are $|00\rangle$, $|10\rangle$, $|20\rangle$ and $\frac{|12\rangle+e^{-i\vartheta_{21}}\alpha|21\rangle}{\sqrt{1+\alpha^2}} =: |\omega\rangle$ as can be seen by applying h to them.

Now, we will examine the ground states on a chain of length $L > 2$. Since our Hamiltonian is frustration free, we know that it already minimizes the energy on every two neighboring sites. We will make use of this fact by constructing the ground states for the chain of length $L+1$ out of the ground states for the chain of length L. For this, we take the ground states on the chain of length L and try a linear combination of this ground states extended with all possibilities for the next site. Then, we apply the Hamiltonian to this linear combination and require the result to be zero since zero is the ground state energy. As we already know the ground states on the chain of length $L = 2$, we will start from those. The ground states for $L = 3$ must then be of the form

$$|\Phi\rangle := |00\rangle \otimes |x_1\rangle + |10\rangle \otimes |x_2\rangle + |20\rangle \otimes |x_3\rangle + |\omega\rangle \otimes |x_4\rangle, \tag{4.14}$$

where

$$|x_i\rangle = c_0^i|0\rangle + c_1^i|1\rangle + c_2^i|2\rangle, \qquad c_0^i, c_1^i, c_2^i \in \mathbb{C}. \tag{4.15}$$

We now have to find solutions of $H|\Phi\rangle \stackrel{!}{=} 0$:

$$H|\Phi\rangle = \underbrace{h_{1,2}|\Phi\rangle}_{=0} + h_{2,3}|\Phi\rangle \tag{4.16}$$

$$= \Big(\mathbb{1}\otimes\mathbb{1}\otimes|1\rangle\langle 1| + \mathbb{1}\otimes\mathbb{1}\otimes|2\rangle\langle 2| - \mathbb{1}\otimes\frac{1}{\alpha^2+1}\Big(|12\rangle + e^{-i\vartheta_{12}}\alpha|21\rangle\Big)\Big(\langle 12| + e^{i\vartheta_{12}}\alpha\langle 21|\Big)\Big)$$
$$\cdot\Big(|00\rangle\otimes|x_1\rangle + |10\rangle\otimes|x_2\rangle + |20\rangle\otimes|x_3\rangle + |\omega\rangle\otimes|x_4\rangle\Big) \tag{4.17}$$

$$= c_1^1|001\rangle + c_2^1|002\rangle + c_1^2|101\rangle + c_2^2|102\rangle + c_1^3|201\rangle + c_2^3|202\rangle$$
$$+ \frac{c_1^4}{\sqrt{1+\alpha^2}}\Big(|121\rangle + e^{-i\vartheta_{21}}\alpha|211\rangle\Big) + \frac{c_2^4}{\sqrt{1+\alpha^2}}\Big(|122\rangle + e^{-i\vartheta_{21}}\alpha|212\rangle\Big) \tag{4.18}$$
$$- \frac{c_1^4}{(1+\alpha^2)^{\frac{3}{2}}}\alpha\Big(e^{i\vartheta_{12}}|112\rangle + \alpha|121\rangle\Big) - \frac{c_2^4}{(1+\alpha^2)^{\frac{3}{2}}}\alpha\Big(e^{i\vartheta_{12}}|212\rangle + \alpha|221\rangle\Big) = 0 \tag{4.19}$$

The equation is satisfied if and only if $c_1^1 = c_2^1 = c_1^2 = c_2^2 = c_1^3 = c_2^3 = c_1^4 = c_2^4 = 0$ because of linear independence. Therefore, the ground states are $|\Phi\rangle = c_0^1|000\rangle + c_0^2|100\rangle + c_0^3|200\rangle + \frac{c_0^4}{\sqrt{1+\alpha^2}}\big(|120\rangle + e^{-i\vartheta_{21}}\alpha|210\rangle\big)$ for arbitrary $c_0^1, c_0^2, c_0^3, c_0^4 \in \mathbb{C}$.

Going on to the chain of length $L = 4$, the ground states are of the form

$$|\Phi_4\rangle := |000\rangle\otimes|x_1\rangle + |100\rangle\otimes|x_2\rangle + |200\rangle|x_3\rangle + \frac{1}{\sqrt{1+\alpha^2}}\Big(|120\rangle + e^{-i\vartheta_{21}}\alpha|210\rangle\Big)\otimes|x_4\rangle, \tag{4.20}$$

where the states $|x_i\rangle$ are defined as in Eq. (4.15). Applying H to $|\Phi_4\rangle$ yields

$$H|\Phi_4\rangle = \underbrace{(h_{1,2}+h_{2,3})|\Phi_4\rangle}_{=0} + h_{3,4}|\Phi_4\rangle \tag{4.21}$$

$$= c_1^1|0001\rangle + c_2^1|0002\rangle + c_1^2|1001\rangle + c_2^2|1002\rangle + c_1^3|2001\rangle + c_2^3|2002\rangle$$
$$+ \frac{c_1^4}{\sqrt{1+\alpha^2}}\Big(|1201\rangle + e^{-i\vartheta_{21}}\alpha|2101\rangle\Big) + \frac{c_2^4}{\sqrt{1+\alpha^2}}\Big(|1202\rangle + e^{-i\vartheta_{21}}\alpha|2102\rangle\Big). \tag{4.22}$$

For fulfilling the condition $H|\Phi_4\rangle = 0$, c_1^i, c_2^i have to be zero $\forall i = 1,2,3,4$ due to linear independence, and the ground states are given by $|\Phi_4\rangle = c_0^1|0000\rangle + c_0^2|1000\rangle + c_0^3|2000\rangle + \frac{c_0^4}{\sqrt{1+\alpha^2}}\big(|1200\rangle + e^{-i\vartheta_{21}}\alpha|2100\rangle\big)$ for any arbitrary $c_0^i \in \mathbb{C}$, $i = 1,2,3,4$.

Now we show that, for a chain with length $L+1$, the ground states are given by $|0\ldots0\rangle$, $|10\ldots0\rangle$, $|20\ldots0\rangle$, and $\frac{1}{\sqrt{1+\alpha^2}}\big(|120\ldots0\rangle + e^{-i\vartheta_{21}}\alpha|210\ldots0\rangle\big)$ if, for the chain with length L,

the ground states are of the same form. We already know that this holds for a chain of length 4. Let the assumption hold for any arbitrary $4 \leq L \in \mathbb{N}$.

The ground states on a chain of length $L+1$ are then given by

$$|\Phi_{L+1}\rangle = |0\dots0\rangle \otimes |x_1\rangle + |10\dots0\rangle \otimes |x_2\rangle + |20\dots0\rangle \otimes |x_3\rangle + \frac{1}{\sqrt{1+\alpha^2}}\Big(|120\dots0\rangle + e^{-i\vartheta_{21}}\alpha|210\dots0\rangle\Big) \otimes |x_4\rangle, \tag{4.23}$$

where $|x_i\rangle$ is defined as in Eq. (4.15). By applying H to $|\Phi_{L+1}\rangle$, we use that H is frustration free:

$$H|\Phi_{L+1}\rangle = \underbrace{\sum_{i=1}^{L-1} h_{i,i+1}|\Phi_{L+1}\rangle}_{=0} + h_{L,L+1}|\Phi_{L+1}\rangle \tag{4.24}$$

$$= c_1^1|0\dots01\rangle + c_2^1|0\dots02\rangle + c_1^2|10\dots01\rangle + c_2^2|10\dots02\rangle + c_1^3|20\dots01\rangle + c_2^3|20\dots02\rangle + \frac{c_1^4}{\sqrt{1+\alpha^2}}\Big(|120\dots01\rangle + e^{-i\vartheta_{21}}\alpha|210\dots01\rangle\Big) + \frac{c_2^4}{\sqrt{1+\alpha^2}}\Big(|120\dots02\rangle + e^{-i\vartheta_{21}}\alpha|210\dots02\rangle\Big) \tag{4.25}$$

$$\stackrel{!}{=} 0$$

Due to linear independence, $c_1^i = c_2^i = 0$, $i = 1,2,3,4$, and therefore $|\Phi_{L+1}\rangle = c_0^1|0\dots0\rangle + c_0^2|10\dots0\rangle + c_0^3|20\dots0\rangle + \frac{c_0^4}{\sqrt{1+\alpha^2}}\left(|120\dots0\rangle + e^{-i\vartheta_{21}}\alpha|210\dots0\rangle\right)$ for any arbitrary c_0^i, $i = 1,2,3,4$. Since the statement holds for $L = 4$ and the inductive step has been performed, the statement holds for any $4 \leq L \in \mathbb{N}$ due to the principle of mathematical induction. Including the cases $L = 2$ and $L = 3$ which we calculated separately, we obtain that for any chain of length $L \geq 2$, there are four ground states which are given by $|0\dots0\rangle, |10\dots0\rangle, |20\dots0\rangle$, and $\frac{1}{\sqrt{1+\alpha^2}}\left(|120\dots0\rangle + e^{-i\vartheta_{21}}\alpha|210\dots0\rangle\right)$.

Now we examine whether we obtain the same ground states by taking the limits of $\psi(B)$ from Eq. (3.6). For that, we apply the commutation relations (3.1) and (3.2) to rearrange the terms of the sum of Eq. (3.6). Hence, we obtain

$$\psi(B) = \sum_{i_1\dots i_L=0}^{2} \mathrm{Tr}(Bv_{i_L}\dots v_{i_1})|i_1\dots i_L\rangle \tag{4.26}$$

$$= \mathrm{Tr}(Bv_0\dots v_0)|0\dots0\rangle + \mathrm{Tr}(Bv_0\dots v_0v_1)\left(\sum_{n=1}^{L-1}\left(\lambda_1 e^{i\vartheta_{10}}\right)^{n-1}|0\dots\underset{\substack{\uparrow\\ \text{position } n}}{1}0\dots0\rangle\right) + \mathrm{Tr}(Bv_0\dots v_0v_2)\left(\sum_{n=1}^{L-1}\left(\lambda_2 e^{i\vartheta_{20}}\right)^{n-1}|0\dots\underset{\substack{\uparrow\\ \text{position } n}}{2}0\dots0\rangle\right) + \mathrm{Tr}(Bv_0\dots v_0v_2v_1)\Bigg(\sum_{n=1}^{L-1}\left(\lambda_1 e^{i\vartheta_{10}}\right)^{n-1}\sum_{m=n}^{L-1}\left(\lambda_2 e^{i\vartheta_{20}}\right)^{m-1}|0\dots\underset{\substack{\uparrow\\ \text{position } n}}{1}0\dots\underset{\substack{\uparrow\\ \text{position } m+1}}{2}0\dots0\rangle + e^{-i\vartheta_{21}}\alpha\sum_{n=1}^{L-1}\left(\lambda_2 e^{i\vartheta_{20}}\right)^{n-1}\sum_{m=n}^{L-1}\left(\lambda_1 e^{i\vartheta_{10}}\right)^{m-1}|0\dots\underset{\substack{\uparrow\\ \text{position } n}}{2}0\dots\underset{\substack{\uparrow\\ \text{position } m+1}}{1}0\dots0\rangle\Bigg), \tag{4.27}$$

and it is not hard to see that

$$\lim_{\substack{\lambda_1\to0,\ \frac{\lambda_1}{\lambda_2}=\alpha\\ \lambda_2\to0}} \psi(B) = \mathrm{Tr}(Bv_0\dots v_0)|0\dots0\rangle + \mathrm{Tr}(Bv_0\dots v_0v_1)|10\dots0\rangle + \mathrm{Tr}(Bv_0\dots v_0v_2)|20\dots0\rangle + \mathrm{Tr}(Bv_0\dots v_0v_2v_1)\left(|120\dots0\rangle + e^{-i\vartheta_{21}}\alpha|210\dots0\rangle\right) \tag{4.28}$$

unless one of $\mathrm{Tr}(Bv_0\dots v_0), \mathrm{Tr}(Bv_0\dots v_0v_1), \mathrm{Tr}(Bv_0\dots v_0v_2)$, and $\mathrm{Tr}(Bv_0\dots v_0v_2v_1)$ vanishes with λ_1 or λ_2. Now, we show that for the matrices defined by Eq. (3.3) and (3.4) for $n = 2$, there always exists a B such that all traces do not vanish. Using the definitions (3.3) and (3.4), we obtain the matrices:

$$v_0 = \begin{pmatrix} e^{i(\vartheta_{01}+\vartheta_{02})} & 0 & 0 & 0 \\ 0 & e^{i\vartheta_{01}}\lambda_2 & 0 & 0 \\ 0 & 0 & e^{i\vartheta_{02}}\lambda_1 & 0 \\ 0 & 0 & 0 & \lambda_1\lambda_2 \end{pmatrix} \tag{4.29}$$

$$v_1 = \begin{pmatrix} 0 & 0 & e^{i\frac{\vartheta_{12}}{2}} & 0 \\ 0 & 0 & 0 & \lambda_2 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{4.30}$$

$$v_2 = \begin{pmatrix} 0 & e^{i\frac{\vartheta_{21}}{2}} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \lambda_1 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{4.31}$$

For

$$B = \begin{pmatrix} c_1 & 0 & 0 & 0 \\ c_2 & 0 & 0 & 0 \\ c_3 & 0 & 0 & 0 \\ \lambda_2^{-1}c_4 & 0 & 0 & 0 \end{pmatrix}, \tag{4.32}$$

where $c_i \in \mathbb{C}$ for $i \in \{1, 2, 3, 4\}$, the traces are

$$\begin{aligned} \mathrm{Tr}(Bv_0\dots v_0) &= c_1 e^{iL(\vartheta_{01}+\vartheta_{02})}, \\ \mathrm{Tr}(Bv_0\dots v_0v_1) &= c_3 e^{i\frac{\vartheta_{12}}{2}} e^{i(L-1)(\vartheta_{01}+\vartheta_{02})}, \\ \mathrm{Tr}(Bv_0\dots v_0v_2) &= c_2 e^{i\frac{\vartheta_{21}}{2}} e^{i(L-1)(\vartheta_{01}+\vartheta_{02})}, \\ \mathrm{Tr}(Bv_0\dots v_0v_2v_1) &= c_4 e^{i\frac{\vartheta_{21}}{2}} e^{i(L-2)(\vartheta_{01}+\vartheta_{02})}. \end{aligned}$$

Since none of them depends on λ_1 or λ_2, none of them vanishes in the limit. For special choices of c_i, $i \in \{1, 2, 3, 4\}$, the vectors $|0\dots0\rangle$, $|10\dots0\rangle$, $|20\dots0\rangle$, and $|120\dots0\rangle + e^{-i\vartheta_{21}}\alpha|210\dots0\rangle$ can be chosen linearly independently. These vectors are identical to those we obtained as ground states of the Hamiltonian (4.13).

Next, we would like to investigate whether a change in n caused by boundary modifications yields a phase transition in this case of dimension $d = 3$. In order to alter n, we can once more make use of the perturbation S introduced in Eq. (4.8). The fact that $[H, S] \neq 0$ in this case is shown by the following counter-example

$$\begin{aligned} HS|120\dots0\rangle = \gamma H|120\dots0\rangle &= \frac{\gamma}{1+\alpha^{-2}}\left(|120\dots0\rangle - e^{-i\vartheta_{21}}\alpha^{-1}|210\dots0\rangle\right) \\ \neq SH|120\dots0\rangle = \frac{1}{1+\alpha^{-2}}S\left(|120\dots0\rangle - e^{-i\vartheta_{21}}\alpha^{-1}|210\dots0\rangle\right) &= \frac{\gamma}{1+\alpha^{-2}}|120\dots0\rangle, \end{aligned}$$

and implies that computations cannot be done as easy as in the case $d = 2$, and thus we will use degenerate perturbation theory to see what happens to the states.

Degenerate Perturbation Theory

Using degenerate perturbation theory allows us to make a statement about the effect of the perturbation S on the ground states and their energies, at least for small perturbation strengths γ. In order to improve readability, we set $\alpha = 1$ and $\vartheta = 0$ in this calculation. Restricted to the eigenspace $\mathbb{E}(0)$ of H corresponding to the eigenvalue zero and represented in the basis $\left(|0\ldots0\rangle, |10\ldots0\rangle, |20\ldots0\rangle, \frac{|120\ldots0\rangle+|210\ldots0\rangle}{\sqrt{2}}\right)$, S is given by

$$S|_{\mathbb{E}(0)} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \gamma & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\gamma}{2} \end{pmatrix}, \tag{4.33}$$

which is already a diagonal matrix. Hence, the ground states of H are the states in zeroth-order perturbation theory, and the energy shifts in first-order perturbation theory can directly be read off from the matrix:

$$\begin{aligned} E^{(1)}_{|0\ldots0\rangle} &= 0 \\ E^{(1)}_{|10\ldots0\rangle} &= \gamma \\ E^{(1)}_{|20\ldots0\rangle} &= 0 \\ E^{(1)}_{\frac{1}{\sqrt{2}}(|120\ldots0\rangle+|210\ldots0\rangle)} &= \frac{\gamma}{2} \end{aligned}$$

Since the states $|0\ldots0\rangle$, $|10\ldots0\rangle$, and $|20\ldots0\rangle$ are also eigenstates of S, the states in zeroth-order perturbation theory and the energies in first-order perturbation theory are exact. However, the vector $|\chi^{(0)}\rangle := \frac{1}{\sqrt{2}}(|120\ldots0\rangle + |210\ldots0\rangle)$ is not an eigenvector of S, so first-order perturbation theory for this state results in

$$\begin{aligned} |\chi^{(1)}\rangle &= |\chi^{(0)}\rangle + \sum_{\substack{m \\ E_m \neq 0}} \frac{\langle m|S|\chi^{(0)}\rangle}{-E_m}|m\rangle \\ &= |\chi^{(0)}\rangle + \frac{\frac{1}{2}\left(\langle 120\ldots0| - \langle 210\ldots0|\right) S \left(|120\ldots0\rangle + |210\ldots0\rangle\right)}{-1} \frac{1}{\sqrt{2}}\left(|120\ldots0\rangle - |210\ldots0\rangle\right) \\ &= \frac{1}{\sqrt{2}}\left(|120\ldots0\rangle + |210\ldots0\rangle\right) - \frac{1}{2\sqrt{2}}\gamma\left(|120\ldots0\rangle - |210\ldots0\rangle\right) \\ &= \frac{1}{\sqrt{2}}\left(\left(1-\frac{\gamma}{2}\right)|120\ldots0\rangle + \left(1+\frac{\gamma}{2}\right)|210\ldots0\rangle\right) \end{aligned}$$

where the vectors $|m\rangle$ indicate the eigenvectors of H. The numerical computation for $\gamma \to 1$ is presented in Fig. 4.3. For $\gamma = 1$ and $L = 6$, we obtain the first excited state as $0.383|120000\rangle + 0.924|210000\rangle$. Thus, the first excited state is expected to lie in the subspace spanned by $|120\ldots0\rangle$ and $|210\ldots0\rangle$ for all γ, and if this assumption is correct, this state can be calculated analytically. The calculated state can then be checked for being an eigenstate what justifies the assumption a posteriori if it is really an eigenstate.

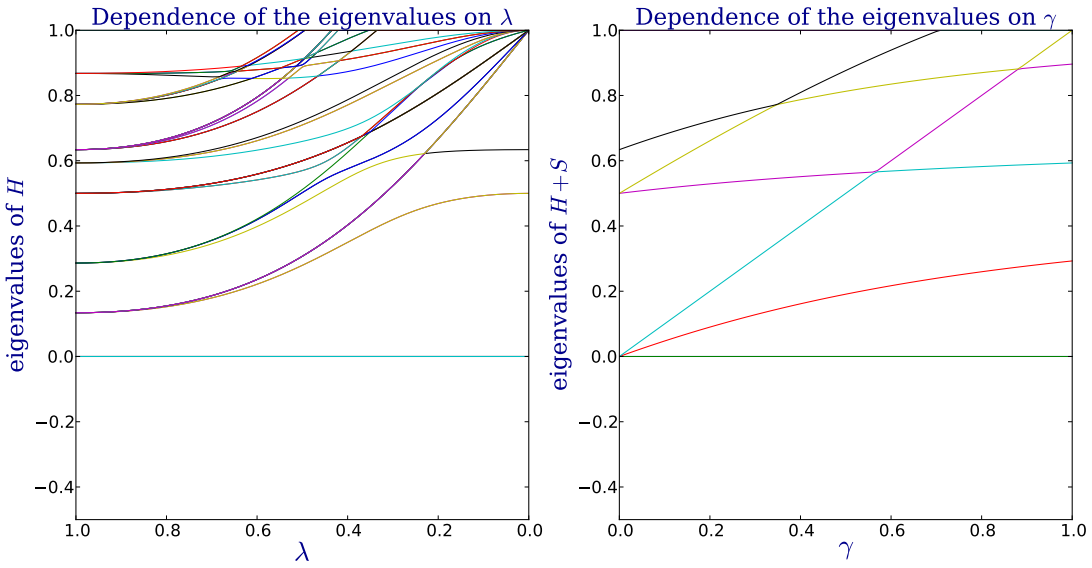

Figure 4.3: The plot on the left shows the eigenvalues of H less than or equal to 1 vs. $\lambda := \lambda_1 = \lambda_2$ (meaning $\alpha = 1$) in the case of length $L = 6$. On the right, the dependence of the eigenvalues ≤ 1 of $H + S$ on γ is depicted. The states $|0\dots0\rangle$ and $|20\dots0\rangle$ are ground states, even for increasing γ. Hence, the ground state is still degenerate. The linearly increasing state is $|10\dots0\rangle$. The forth former ground state (red curve) is the one we assume to lie in the subspace spanned by $|120\dots0\rangle$ and $|210\dots0\rangle$.

Exact Calculation

As just mentioned, we may be able to calculate the first excited state exactly. For that, we will use the assumption that the first excited state lies in the vector space $\text{span}\{|120\dots0\rangle, |210\dots0\rangle\}$ which is also generated by the eigenvectors $|\chi_1\rangle := \frac{|120\dots0\rangle+|210\dots0\rangle}{\sqrt{2}}$ and $|\chi_2\rangle := \frac{|120\dots0\rangle-|210\dots0\rangle}{\sqrt{2}}$ of H. Then, we check whether the computed state is really an eigenstate since if it is, the assumption is justified.

The vectors $|\chi_1\rangle$ and $|\chi_2\rangle$ are mapped by H and S to

$$\begin{aligned} H|\chi_1\rangle &= 0, & H|\chi_2\rangle &= |\chi_2\rangle \\ S|\chi_1\rangle &= \frac{\gamma}{\sqrt{2}}|120\dots0\rangle, & S|\chi_2\rangle &= \frac{\gamma}{\sqrt{2}}|120\dots0\rangle \end{aligned}$$

so that the matrix elements are given by

$$\langle X|(H+S)|\chi_1\rangle = \begin{cases} \frac{\gamma}{2} & \text{for } |X\rangle = |\chi_1\rangle \text{ or } |X\rangle = |\chi_2\rangle \\ 0 & \text{otherwise} \end{cases}$$

$$\langle X|(H+S)|\chi_2\rangle = \begin{cases} \frac{\gamma}{2} & \text{for } |X\rangle = |\chi_1\rangle \\ 1+\frac{\gamma}{2} & \text{for} |X\rangle = |\chi_2\rangle \\ 0 & \text{otherwise} \end{cases}.$$

As $H + S$ is self-adjoint, the only non-vanishing matrix elements are

$$M := \begin{pmatrix} \frac{\gamma}{2} & \frac{\gamma}{2} \\ \frac{\gamma}{2} & 1+\frac{\gamma}{2} \end{pmatrix}.$$

Diagonalizing M leads to the characteristic polynomial

$$\det\begin{pmatrix} \frac{\gamma}{2}-x & \frac{\gamma}{2} \\ \frac{\gamma}{2} & 1+\frac{\gamma}{2}-x \end{pmatrix} = x^2-(\gamma+1)x+\frac{\gamma}{2}, \tag{4.34}$$

from which the energies

$$x_1 = \frac{\gamma+1}{2}+\frac{1}{2}\sqrt{\gamma^2+1} \tag{4.35}$$

$$x_2 = \frac{\gamma+1}{2}-\frac{1}{2}\sqrt{\gamma^2+1} \tag{4.36}$$

can be extracted. These do not depend on the length L of the chain, because for larger L, there are only zeros on sites $3,4,\ldots,L-1$ which do not contribute to the energy. Therefore, the only sites relevant for the energy are the first three sites.

We are interested in the eigenstate with the smaller eigenvalue $x_2 \in (0, 1-\frac{1}{\sqrt{2}})$ for $\gamma \in (0,1)$, and since $1-\frac{1}{\sqrt{2}} < 0.5$, this eigenvalue belongs to the first excited state as can be seen in the numerical result in Fig. 4.3. This state is given by $|v\rangle = N\left(\gamma|\chi_1\rangle + (1-\sqrt{1+\gamma^2})|\chi_2\rangle\right)$. Finally, normalization leads to the first excited state

$$|v\rangle = \frac{1}{2\sqrt{\gamma^2+1-\sqrt{\gamma^2+1}}}\left[\left(1-\sqrt{\gamma^2+1}+\gamma\right)|120\ldots0\rangle + \left(\sqrt{\gamma^2+1}-1+\gamma\right)|210\ldots0\rangle\right].$$

A simple calculation shows that $H|v\rangle = \left(\frac{\gamma+1}{2}-\frac{1}{2}\sqrt{\gamma^2+1}\right)|v\rangle$. Accordingly, the assumption that the first excited state lies in the subspace generated by $|120\ldots0\rangle$ and $|210\ldots0\rangle$ for all γ was justified.

Let us now have a look at the Hamiltonian for $\gamma = 1$ which is then given by

$$H' := H + S \tag{4.37}$$

$$= \sum_{i=1}^{L}|1\rangle\langle1|_i + \sum_{i=2}^{L}|2\rangle\langle2|_i - \frac{1}{1+\alpha^2}\sum_{i=1}^{L-1}\left(\left(|12\rangle+e^{-i\vartheta_{21}}\alpha|21\rangle\right)\left(\langle12|+e^{i\vartheta_{21}}\alpha\langle21|\right)\right)_{i,i+1}. \tag{4.38}$$

As computed previously, it has the ground states $|0\ldots0\rangle$ and $|20\ldots0\rangle$. Hence, the ground state is twofold degenerate, and this Hamiltonian belongs to $n=1$, $d=3$, albeit not of the desired form

$$\sum_{i=1}^{L}|1\rangle\langle1|_i + \sum_{i=2}^{L-1}|2\rangle\langle2|_i \tag{4.39}$$

because it still contains a two-particle interaction. Nevertheless, it serves as an example of a way to force an alteration of n only by adding a modification to the boundary. But even in this case, the change of the ground state space has only an effect on the edge of the system and the bulk remains continuous.

Adding a Perturbation Acting on Particle Type 2

Next, we analyze the transition $n = 1 \mapsto n = 0$ for dimension $d = 3$. Therefore, we turn on a perturbation acting on particle type 2 on the first site with perturbation strength β

$$W := \beta|2\rangle\langle 2| \otimes \mathbb{1}, \qquad \beta > 0, \tag{4.40}$$

yielding the Hamiltonian

$$\begin{aligned} H'' &:= H' + W \qquad (4.41)\\ &= \sum_{i=1}^{L} |1\rangle\langle 1|_i + \sum_{i=2}^{L} |2\rangle\langle 2|_i + \beta|2\rangle\langle 2|_1 \\ &\quad - \frac{1}{1+\alpha^2} \sum_{i=1}^{L-1} \Big(\Big(|12\rangle + e^{-i\vartheta_{21}}\alpha|21\rangle \Big) \Big(\langle 12| + e^{i\vartheta_{21}}\alpha\langle 21| \Big) \Big)_{i,i+1}. \qquad (4.42) \end{aligned}$$

Calculating the expectation values of the ground states of H'' shows that the ground state $|20\ldots0\rangle$ gains the energy β, and therefore no longer belongs to the ground state space. Since $|20\ldots0\rangle$ is an eigenstate of W, the energy increases linearly with the perturbation scale β as can be seen in Fig. 4.4. So $|0\ldots0\rangle$ is the only ground state of the Hamiltonian (4.41). As a result, this Hamiltonian belongs to the case $n = 0$ and $d = 3$. But even for $\beta = 1$, the Hamiltonian is not translation invariant.

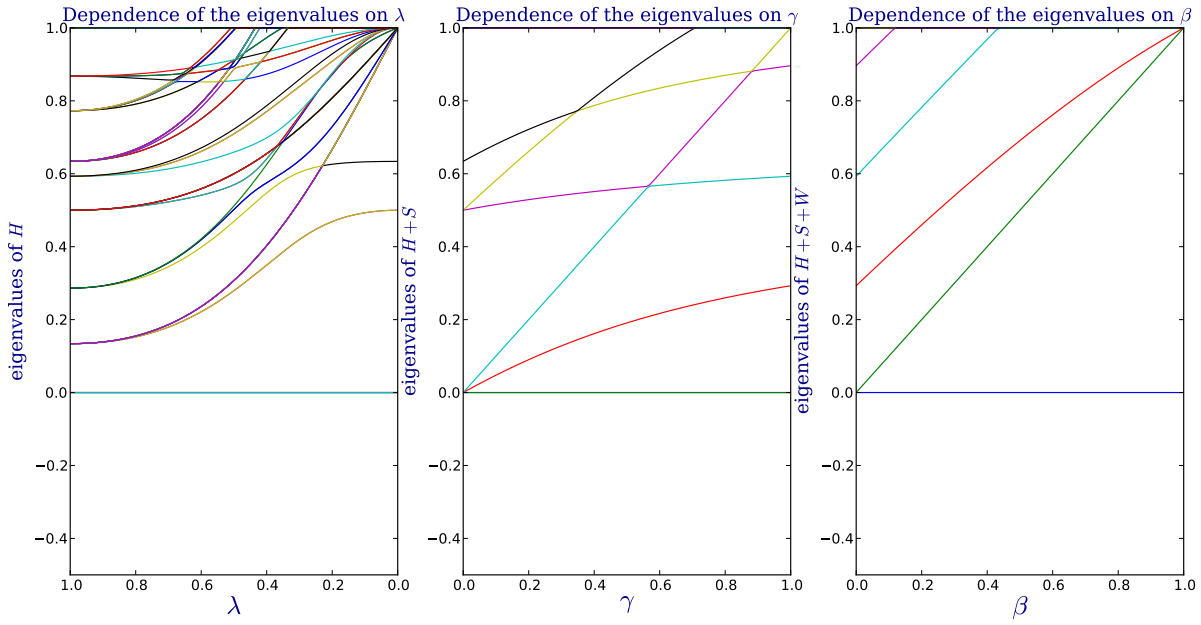

Figure 4.4: On the left, the figure shows the dependence of the eigenvalues of $H = \sum_{i=2}^{L}(|1\rangle\langle 1|_i + |2\rangle\langle 2|_i) - \frac{1}{2}\sum_{i=1}^{L-1}((|12\rangle + |21\rangle)(\langle 12| + \langle 21|))_{i,i+1}$ on $\lambda := \lambda_1 = \lambda_2$ in the case $L = 6$. Only the lower part of the spectrum is plotted since we are interested in the energy of the ground states and the first excited states. In the middle we see how the eigenvalues of $H + S = \sum_{i=1}^{L}|1\rangle\langle 1|_i + \sum_{i=2}^{L}|2\rangle\langle 2|_i - \frac{1}{2}\sum_{i=1}^{L-1}((|12\rangle + |21\rangle)(\langle 12| + \langle 21|))_{i,i+1}$ depend on γ. On the right, the plot depicts the behavior of the eigenvalues of $H+S+W = \sum_{i=1}^{L}|1\rangle\langle 1|_i + \sum_{i=2}^{L}|2\rangle\langle 2|_i + \beta|2\rangle\langle 2|_1 - \frac{1}{2}\sum_{i=1}^{L-1}((|12\rangle + |21\rangle)(\langle 12| + \langle 21|))_{i,i+1}$ depending on β. It shows that the ground states split up and the energy of the new first excited state $|20\ldots0\rangle$ increases linearly with β. The remaining ground state $|0\ldots0\rangle$ remains constant at zero energy.

Adding a Perturbation Acting on Both Particle Types

So far we have only changed n by one; in the following we strive to examine the situation when the number n of particle types occurring in the ground states is altered by 2, i.e. from 2 to 0. In order to do this, we make an ansatz containing a perturbation which acts on both particle types on the left boundary:

$$V = \delta \left(|1\rangle\langle 1| \otimes \mathbb{1}_{L-1} + |2\rangle\langle 2| \otimes \mathbb{1}_{L-1} \right), \qquad \delta > 0 \tag{4.43}$$

where $\mathbb{1}_{L-1}$ acts on $(L-1)$ sites, and δ denotes the perturbation strength. The commutator of H and V vanishes, which can be proven as follows:

h can be decomposed into a diagonal part and a non-diagonal part:

$$h = \underbrace{|01\rangle\langle 01| + |02\rangle\langle 02| + |11\rangle\langle 11| + |22\rangle\langle 22|}_{=:h_{\mathrm{D}}} + \underbrace{\frac{1}{1+\alpha^2}\left(\alpha|12\rangle - e^{-i\vartheta_{21}}|21\rangle\right)\left(\alpha\langle 12| - e^{i\vartheta_{21}}\langle 21|\right)}_{=:h_{\mathrm{N}}}$$

The diagonal part commutes with V since V is diagonal as well, thus

$$[h, V] = \underbrace{[h_{\mathrm{D}}, V]}_{=0} + [h_{\mathrm{N}}, V].$$

The remaining commutator $[h_{\mathrm{N}}, V]$ also vanishes what can be seen by

$$\begin{aligned}
h_{\mathrm{N}} V &= \left(\frac{1}{1+\alpha^2}\left(\alpha|12\rangle - e^{-i\vartheta_{21}}|21\rangle\right)\left(\alpha\langle 12| - e^{i\vartheta_{21}}\langle 21|\right)\right)\delta\left(|1\rangle\langle 1| \otimes \mathbb{1} + |2\rangle\langle 2| \otimes \mathbb{1}\right) \\
&= \delta\left(\frac{\alpha}{1+\alpha^2}\left(\alpha|12\rangle - e^{-i\vartheta_{21}}|21\rangle\right)\langle 12| + \frac{1}{1+\alpha^2}\left(|21\rangle - e^{i\vartheta_{21}}\alpha|12\rangle\right)\langle 21|\right) \\
= V h_{\mathrm{N}} &= \delta\left(|1\rangle\langle 1| \otimes \mathbb{1} + |2\rangle\langle 2| \otimes \mathbb{1}\right)\left(\frac{1}{1+\alpha^2}\left(\alpha|12\rangle - e^{-i\vartheta_{21}}|21\rangle\right)\left(\alpha\langle 12| - e^{i\vartheta_{21}}\langle 21|\right)\right) \\
&= \delta\left(\frac{\alpha}{1+\alpha^2}|12\rangle\left(\alpha\langle 12| - e^{i\vartheta_{21}}\langle 21|\right) + \frac{1}{1+\alpha^2}|21\rangle\left(\langle 21| - e^{-i\vartheta_{21}}\alpha\langle 12|\right)\right) \\
&= \delta\left(\frac{\alpha}{1+\alpha^2}\left(\alpha|12\rangle - e^{-i\vartheta_{21}}|21\rangle\right)\langle 12| + \frac{1}{1+\alpha^2}\left(|21\rangle - e^{i\vartheta_{21}}\alpha|12\rangle\right)\langle 21|\right).
\end{aligned}$$

So $[h, V] = 0$, yielding for the total Hamiltonian

$$\begin{aligned}
[H, V] &= \sum_{x=1}^{L-1} [h_{x,x+1}, V] \\
&= [h, \delta\left(|1\rangle\langle 1| \otimes \mathbb{1} + |2\rangle\langle 2| \otimes \mathbb{1}\right)] \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1} + \sum_{x=2}^{L-1} [h_{x,x+1}, V] \\
&= \sum_{x=2}^{L-1} [\underbrace{\mathbb{1} \otimes \cdots \otimes \mathbb{1}}_{x-1 \geq 1 \text{ times}} \otimes h \otimes \mathbb{1} \otimes \cdots \mathbb{1}, V] = 0,
\end{aligned}$$

which is also confirmed by the linear increase in δ as plotted in Fig. 4.5. The ground states $|0\ldots0\rangle$, $|10\ldots0\rangle$, $|20\ldots0\rangle$ and $\frac{|120\ldots0\rangle + e^{-i\vartheta_{21}}\alpha|210\ldots0\rangle}{\sqrt{1+\alpha^2}}$ are already eigenstates of the perturbation V. Therefore, the eigenvalues can be summed and since three of the former four ground states get a positive energy, the four-dimensional vector space of the ground states becomes a one-dimensional subspace spanned by $|0\ldots0\rangle$. Due to the fact that a change only happens at the boundary, the bulk of the system again remains unchanged. Thus, we obtain no phase transition.

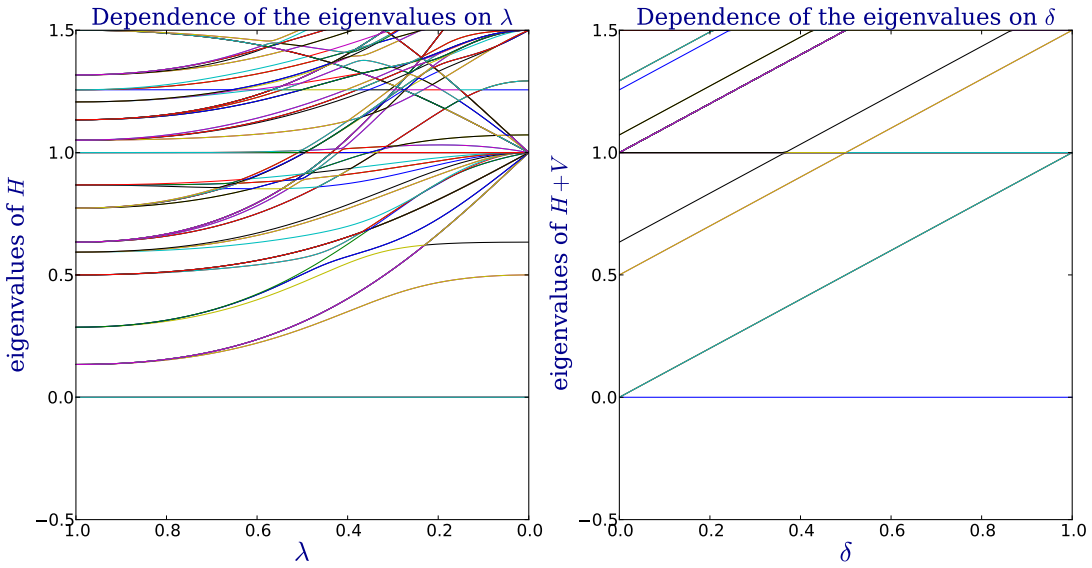

Figure 4.5: On the left, the eigenvalues of H less than or equal to 1.5 are shown as functions of $\lambda := \lambda_1 = \lambda_2$. The plot on the right depicts the dependence of the eigenvalues of $H + V$ on δ. The linearly increasing curves indicate that $[H, V] = 0$. For $\delta > 0$, the only remaining ground state is $|0 \dots 0\rangle$; the states $|10 \dots 0\rangle, |20 \dots 0\rangle$, and $\frac{1}{2}(|120 \dots 0\rangle) + e^{-i\vartheta_{21}}|210 \dots 0\rangle$ increase with δ. Therefore, the degeneracy of the ground state is removed.

In this case, the Hamiltonian belonging to $n = 0$ and $d = 3$ where we set $\delta = 1$ is given by

$$H' = H + V \tag{4.44}$$

$$= \sum_{i=1}^{L} |1\rangle\langle 1|_i + \sum_{i=1}^{L} |2\rangle\langle 2|_i - \frac{1}{1+\alpha^2} \sum_{i=1}^{L-1} \left(\left(|12\rangle + e^{-i\vartheta_{21}} \alpha |21\rangle \right) \left(\langle 12| + e^{i\vartheta_{21}} \alpha \langle 21| \right) \right)_{i,i+1}, \tag{4.45}$$

which, again, is not translation invariant.

4.2.2 Taking the Limits One After The Other

In the last section, we investigated the behavior of the PVBS-model when taking the limits $\lambda_1 \to 0$ and $\lambda_2 \to 0$ with constant ratio $\frac{\lambda_1}{\lambda_2}$. In the following, we examine the case where the limits $\lambda_1 \to 0$ and $\lambda_2 \to 0$ are taken consecutively, i.e. a particle of type 1 binds to the left edge before particles of type two do.

Taking the limits this way, the Hamiltonian acting on two neighboring sites is given by:

$$\begin{aligned}
\lim_{\lambda_2\to 0}\lim_{\lambda_1\to 0} h &= \lim_{\lambda_2\to 0}\lim_{\lambda_1\to 0}\Bigg[\frac{1}{1+\lambda_1^2}\Big(|01\rangle - e^{-i\vartheta_{10}}\lambda_1|10\rangle\Big)\Big(\langle 01| - e^{i\vartheta_{10}}\lambda_1\langle 10|\Big) + |11\rangle\langle 11| \\
&+ \frac{1}{1+\lambda_2^2}\Big(|02\rangle - e^{-i\vartheta_{20}}\lambda_2|20\rangle\Big)\Big(\langle 02| - e^{i\vartheta_{20}}\lambda_2\langle 20|\Big) + |22\rangle\langle 22| \\
&+ \frac{1}{\lambda_1^2+\lambda_2^2}\Big(\lambda_1|12\rangle - e^{-i\vartheta_{21}}\lambda_2|21\rangle\Big)\Big(\lambda_1\langle 12| - e^{i\vartheta_{21}}\lambda_2\langle 21|\Big)\Bigg] \\
&= \lim_{\lambda_2\to 0}\Big[|01\rangle\langle 01| + |11\rangle\langle 11| + \frac{1}{1+\lambda_2^2}\Big(|02\rangle - e^{-i\vartheta_{20}}\lambda_2|20\rangle\Big)\Big(\langle 02| - e^{i\vartheta_{20}}\lambda_2\langle 20|\Big) \\
&+ |22\rangle\langle 22| + |21\rangle\langle 21|\Big] \\
&= |01\rangle\langle 01| + |11\rangle\langle 11| + |02\rangle\langle 02| + |22\rangle\langle 22| + |21\rangle\langle 21| \\
&= \mathbb{1}\otimes|1\rangle\langle 1| + \mathbb{1}\otimes|2\rangle\langle 2| - |12\rangle\langle 12|
\end{aligned}$$

Hence, the Hamiltonian

$$H = \sum_{i=1}^{L-1} h_{i,i+1} = \sum_{i=1}^{L-1}\left(|1\rangle\langle 1|_{i+1} + |2\rangle\langle 2|_{i+1} - |12\rangle\langle 12|_{i,i+1}\right) \tag{4.46}$$

acting on the entire chain is already diagonal if it is written in the product basis. The ground state space is spanned by $|0\ldots 0\rangle$, $|10\ldots 0\rangle$, $|20\ldots 0\rangle$, and $|120\ldots 0\rangle$.

In order to verify that we obtain the same ground states by starting with $\psi(B)$, we take the limits of Eq. (4.27):

$$\begin{aligned}
\lim_{\lambda_2\to 0}\lim_{\lambda_1\to 0}\psi(B) = \lim_{\lambda_2\to 0}\Bigg(&\mathrm{Tr}(Bv_0\ldots v_0)|0\ldots 0\rangle + \mathrm{Tr}(Bv_0\ldots v_0v_1)|10\ldots 0\rangle \\
&+ \mathrm{Tr}(Bv_0\ldots v_0v_2)\left(\sum_{n=1}^{L-1}\left(\lambda_2 e^{i\vartheta_{20}}\right)^{n-1}|0\ldots \underset{\substack{\uparrow\\ \text{position } n}}{020}\ldots 0\rangle\right) \\
&+ \mathrm{Tr}(Bv_0\ldots v_0v_2v_1)\left(\sum_{m=1}^{L-1}\left(\lambda_2 e^{i\vartheta_{20}}\right)^{m-1}|10\ldots \underset{\substack{\uparrow\\ \text{position } m+1}}{020}\ldots 0\rangle\right)\Bigg) \\
= &\,\mathrm{Tr}(Bv_0\ldots v_0)|0\ldots 0\rangle + \mathrm{Tr}(Bv_0\ldots v_0v_1)|10\ldots 0\rangle \\
&+ \mathrm{Tr}(Bv_0\ldots v_0v_2)|20\ldots 0\rangle + \mathrm{Tr}(Bv_0\ldots v_0v_2v_1)|120\ldots 0\rangle
\end{aligned}$$

This only holds if $\mathrm{Tr}(Bv_0\ldots v_0), \mathrm{Tr}(Bv_0\ldots v_0v_1), \mathrm{Tr}(Bv_0\ldots v_0v_2)$, and $\mathrm{Tr}(Bv_0\ldots v_0v_2v_1)$ do not vanish in the limit. Since we are explicitly able to provide an appropriate B (cf. Eq. (4.32)), we know that a B exists such that the traces do not vanish. As this B allows us to obtain the vectors $|0\ldots 0\rangle, |10\ldots 0\rangle, |20\ldots 0\rangle$, and $|120\ldots 0\rangle$ separately, the ground state space is four-dimensional. These states are equal to those we found as ground states of the Hamiltonian (4.46) directly.

Since $h_{i,i+1}$ is diagonal, it is obvious that $[h_{i,i+1}, h_{j,j+1}] = 0 \quad \forall i,j = 1,2,\ldots,L-1$. Therefore, after taking the limits $\lambda_1 \to 0$ and $\lambda_2 \to 0$, the eigenvalues of H become integers as can be seen in Fig. 4.6.

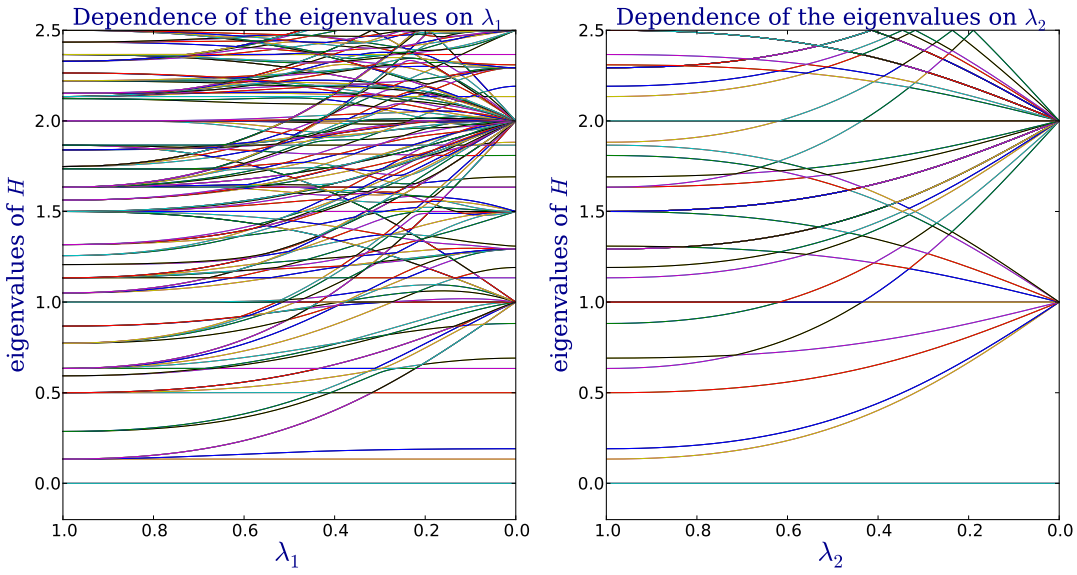

Figure 4.6: The plot on the left depicts the eigenvalues of H dependent on λ_1 where $\lambda_2 = 1 - \frac{1}{1000}$, exemplarily in the case of chain length $L = 6$. Here, only the eigenvalues which are less then or equal to 2.5 are shown for clarity. On the right, the dependence of the eigenvalues of H on λ_2 where $\lambda_1 = 0$ is shown. For $\lambda_2 \to 0$, the eigenvalues become integers; this indicates that for $\lambda_1 \to 0$ and then $\lambda_2 \to 0$ the $h_{i,i+1}$ commute with each other.

Adding a Perturbation Acting on Both Particle Types

Now, let us change n from 2 to 0 by adding the perturbation V acting on the first site and both types of particles (cf. Eq. (4.43)) to the Hamiltonian:

$$H' = H + V = \sum_{i=1}^{L-1} \left(|1\rangle\langle 1|_{i+1} + |2\rangle\langle 2|_{i+1} - |12\rangle\langle 12|_{i,i+1}\right) + \delta\left(|1\rangle\langle 1| \otimes \mathbb{1} + |2\rangle\langle 2| \otimes \mathbb{1}\right) \tag{4.47}$$

$$\xrightarrow{\delta \to 1} \sum_{i=1}^{L} \left(|1\rangle\langle 1|_i + |2\rangle\langle 2|_i\right) - \sum_{i=1}^{L-1} |12\rangle\langle 12|_{i,i+1} \tag{4.48}$$

The states $|10\ldots0\rangle$, $|20\ldots0\rangle$ and $|120\ldots0\rangle$ are eigenstates of V with eigenvalue δ. Hence, their energies increase with δ, and they do not belong to the space of ground states anymore which means that the gap vanished. The only ground state left is $|0\ldots0\rangle$ and the Hamiltonian belongs to $n = 0$ although it does not have the desired, translation invariant form (4.1).

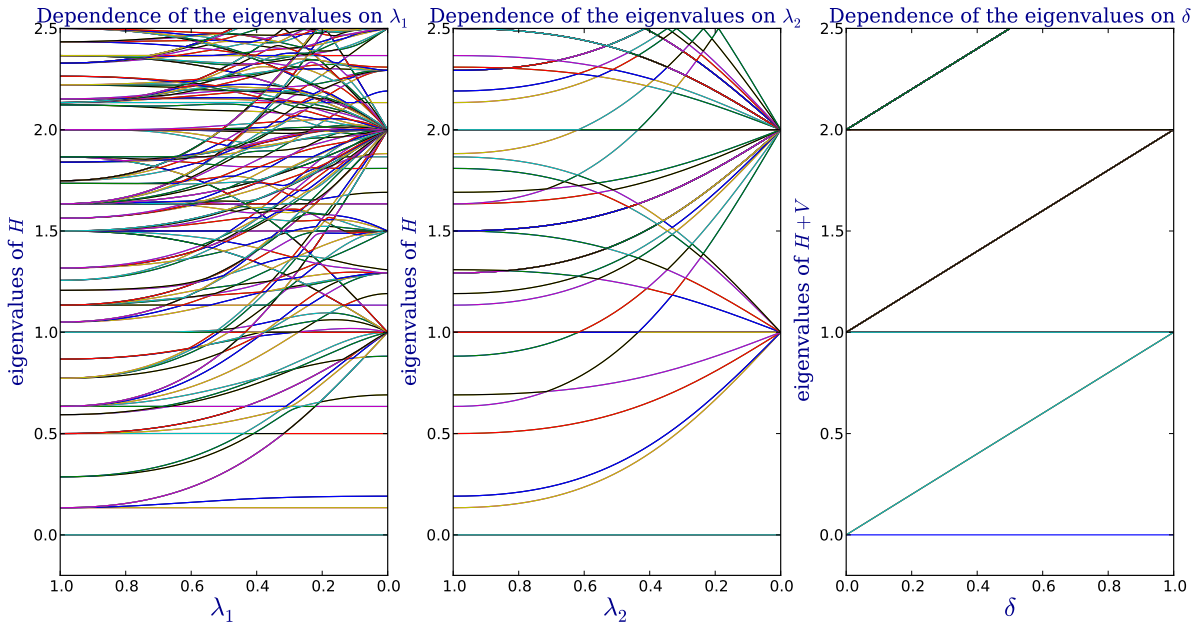

Figure 4.7: The figure shows (exemplarily for $L = 6$) the eigenvalues of H dependent on λ_1 for $\lambda_2 = 1$ on the left, and dependent on λ_2 for $\lambda_1 = 0$ in the middle. The plot on the right depicts the dependence of the eigenvalues of $H + V$ on δ. The linear increase indicates that $[H, V] = 0$. What cannot be seen explicitly is that the states $|10\ldots0\rangle, |20\ldots0\rangle$ and $|120\ldots0\rangle$ increase with δ, so the remaining ground state is only $|0\ldots0\rangle$.

Adding a Perturbation Acting Only on One Particle Type

By taking the limit $\lambda_1 \to 0$ before the limit $\lambda_2 \to 0$, particle type 1 is given a special role. And though this was not important yet, it becomes relevant for the change $n = 2 \mapsto n = 1$ because it makes a difference whether the perturbation on the first site acts on particle type 1 or particle type 2.

To see this, we consider the perturbation acting on particle type 1:

$$S_1 := \gamma_1 |1\rangle\langle 1| \otimes \mathbb{1}, \qquad \gamma_1 > 0. \tag{4.49}$$

The ground states of the Hamiltonian

$$H' = H + S_1 = \sum_{i=1}^{L-1} \left(|1\rangle\langle 1|_{i+1} + |2\rangle\langle 2|_{i+1} - |12\rangle\langle 12|_{i,i+1} \right) + \gamma_1 |1\rangle\langle 1| \otimes \mathbb{1} \tag{4.50}$$

are given by $|0\ldots0\rangle$ and $|20\ldots0\rangle$ such that the Hamiltonian belongs to $n = 1$. For $\gamma_1 = 1$, the Hamiltonian can even be written in the form

$$H' = \sum_{i=1}^{L} |1\rangle\langle 1|_i + \sum_{i=1}^{L-1} \left(|2\rangle\langle 2|_{i+1} - |12\rangle\langle 12|_{i,i+1} \right). \tag{4.51}$$

In order to change the number of particle types occurring in the ground states from $n = 1$ to $n = 0$, a perturbation acting on particle type 2 is added to the first site:

$$S_2 := \gamma_2 |2\rangle\langle 2| \otimes \mathbb{1}, \qquad \gamma_2 > 0 \tag{4.52}$$

$$H'' := H + S_1 + S_2 = \sum_{i=1}^{L} |1\rangle\langle 1|_i + \sum_{i=1}^{L-1} \left(|2\rangle\langle 2|_{i+1} - |12\rangle\langle 12|_{i,i+1}\right) + \gamma_2 |2\rangle\langle 2| \otimes \mathbb{1} \tag{4.53}$$

This Hamiltonian belongs to $n = 0$ since the only ground state is given by $|0 \dots 0\rangle$. For $\gamma_2 = 1$, we obtain the same Hamiltonian (4.48) as in the case $n = 2 \mapsto n = 0$.

However, if the perturbation acting on particle type 2 (Eq. (4.52)) is added first, we obtain the following Hamiltonian

$$H' = H + S_2 = \sum_{i=1}^{L-1} \left(|1\rangle\langle 1|_{i+1} + |2\rangle\langle 2|_{i+1} - |12\rangle\langle 12|_{i,i+1}\right) + \gamma_2 |2\rangle\langle 2| \otimes \mathbb{1} \tag{4.54}$$

with ground states $|0 \dots 0\rangle$, $|10 \dots 0\rangle$ and $|120 \dots 0\rangle$. That is interesting since, in this case, the degeneracy of the ground state is three and not given by 2^n where $n \in \mathbb{N}$. Thus, the Hamiltonian H' given in Eq. (4.54) does not fit to the scheme of PVBS.

4.2.3 Manipulations on the Entire Chain

The Hamiltonians we obtained in order to change n read for $\alpha = \text{const.}$,

$$H'_{n=2\to n=1} = \sum_{i=1}^{L} |1\rangle\langle 1|_i + \sum_{i=2}^{L} |2\rangle\langle 2|_i - \frac{1}{1+\alpha^2} \sum_{i=1}^{L-1} \left(\left(|12\rangle + e^{-i\vartheta_{21}}\alpha|21\rangle\right)\left(\langle 12| + e^{i\vartheta_{21}}\alpha\langle 21|\right)\right)_{i,i+1} \tag{4.55}$$

$$H'_{n=2\to n=0} = \sum_{i=1}^{L} |1\rangle\langle 1|_i + \sum_{i=1}^{L} |2\rangle\langle 2|_i - \frac{1}{1+\alpha^2} \sum_{i=1}^{L-1} \left(\left(|12\rangle + e^{-i\vartheta_{21}}\alpha|21\rangle\right)\left(\langle 12| + e^{i\vartheta_{21}}\alpha\langle 21|\right)\right)_{i,i+1}, \tag{4.56}$$

and those for $\lambda_1 \to 0$ before $\lambda_2 \to 0$, read

$$H'_{n=2\to n=0} = \sum_{i=1}^{L} |1\rangle\langle 1|_i + \sum_{i=1}^{L} |2\rangle\langle 2|_i - \sum_{i=1}^{L-1} |12\rangle\langle 12|_{i,i+1} \tag{4.57}$$

$$H'_{n=2\to n=1} = \sum_{i=1}^{L} |1\rangle\langle 1|_i + \sum_{i=1}^{L-1} |2\rangle\langle 2|_i - \sum_{i=1}^{L-1} |12\rangle\langle 12|_{i,i+1}. \tag{4.58}$$

They all have in common that there are still terms of a two-particle interaction. Now, we try to artificially eliminate them.

This can be achieved by adding terms like

$$w_{i,i+1} = \left(\frac{\varepsilon}{2}\left(|12\rangle + e^{-i\vartheta_{21}}\alpha|21\rangle\right)\left(\langle 12| + e^{i\vartheta_{21}}\alpha\langle 21|\right)\right)_{i,i+1}, \qquad i = 1, \dots, L-1 \tag{4.59}$$

in the cases where $\alpha = \text{const.}$, and taking the limit $\varepsilon \to 1$. In the case $n = 2 \mapsto n = 0$ and $n = 2 \mapsto n = 1$, respectively, this yields the Hamiltonian

$$H''_{n=2\to n=0} = \sum_{i=1}^{L} \left(|1\rangle\langle 1|_i + |2\rangle\langle 2|_i\right) \tag{4.60}$$

and

$$H''_{n=2\to n=1} = \sum_{i=1}^{L} |1\rangle\langle 1|_i + \sum_{i=2}^{L} |2\rangle\langle 2|_i. \tag{4.61}$$

These are the forms we desired for the Hamiltonian if $d > n+1$. As can be seen in Fig. (4.8), the added terms leave the gap open so the ground states remain the same, and therefore the system does not undergo a phase transition.

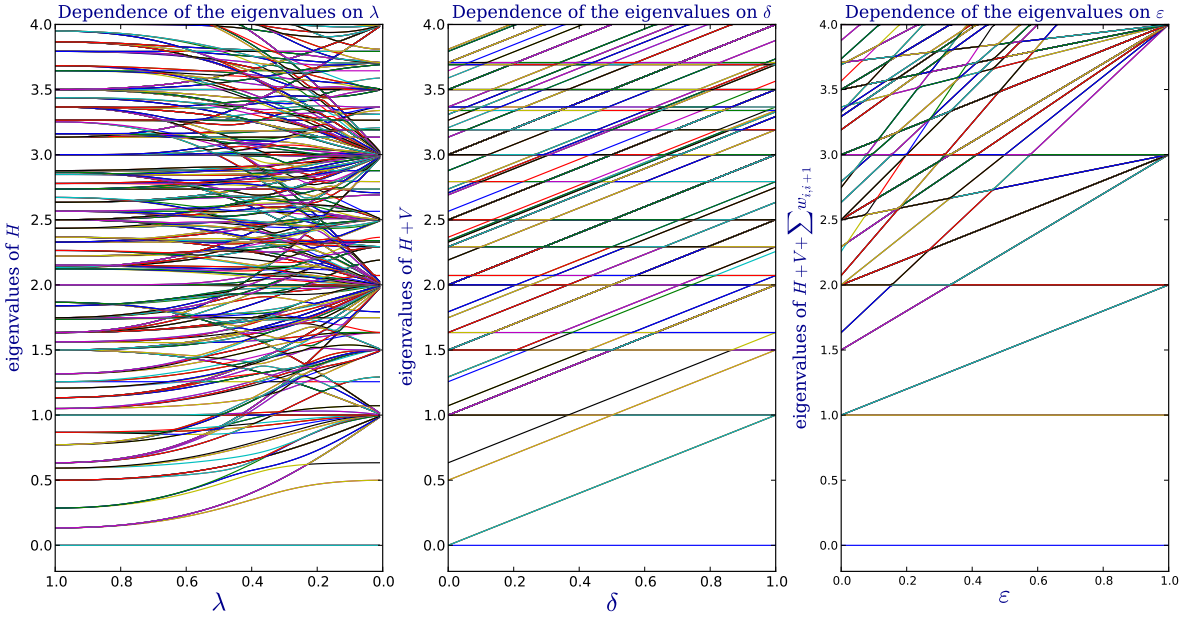

Figure 4.8: On the left, a part of the spectrum of H vs. $\lambda := \lambda_1 = \lambda_2$ for $L = 6$ is shown. The linear dependence of the eigenvalues of $H + V$ on the perturbation strength δ is depicted in the middle. On the right, we see how the eigenvalues of $H + V + \sum_{i=1}^{L-1} w_{i,i+1}$ depend on ε. For $\varepsilon \to 1$, all eigenvalues become non-negative integers.

In the case where $\lambda_1 \to 0$ before $\lambda_2 \to 0$, the terms of a two-particle interaction still remain on the entire chain, but they are not entangled like in the case of constant ratio α. So we can obtain the Hamiltonian (4.60) or (4.61) by adding a two-particle interaction like

$$w'_{i,i+1} = \rho|12\rangle\langle 12|_{i,i+1}, \qquad i = 1, \ldots, L-1 \tag{4.62}$$

and taking the limit $\rho \to 1$.

Since the operators $w_{i,i+1}$ and $w'_{i,i+1}$ represent two-particle interactions, it might be difficult to realize them in an experiment. Moreover, they have to be provided on the entire chain. Thus, for $n = 2$ it is not possible to obtain a Hamiltonian which has the same effect on every site, except the first one in the case $n = 2 \mapsto n = 1$, only by modifying the boundary. However, in chapter 6, we will develop a new modified form of PVBS which is capable of avoiding this problem.

4.3 Moving Particles from One Boundary to the Other

Coming back to the case of dimension $d = 2$ and $n = 1$, we now try to examine whether it is possible to move the particle from one edge to the other continuously. For that, we construct a path by superposing the Hamiltonian h as a function of λ or λ^{-1}, respectively, and using $\theta \in [0, 1]$ as an interpolation parameter. For readability, ϑ_{01} is fixed to zero. In order to send the particle to the edges, we take the limit $\lambda \to 0$:

$$\begin{aligned}\lim_{\lambda\to 0}\left[\theta h(\lambda) + (1-\theta)h(\lambda^{-1})\right] &= \lim_{\lambda\to 0}\Big[\frac{1}{1+\lambda^2}\left(\lambda^2|01\rangle\langle 01| - \lambda|01\rangle\langle 10| - \lambda|10\rangle\langle 01| + |10\rangle\langle 10|\right)\\ &\quad + |11\rangle\langle 11| + \frac{\theta}{1+\lambda^2}\left((1-\lambda^2)|01\rangle\langle 01| + (\lambda^2-1)|10\rangle\langle 10|\right)\Big]\\ &= |11\rangle\langle 11| + |10\rangle\langle 10| + \theta\left(|01\rangle\langle 01| - |10\rangle\langle 10|\right)\\ &= (1-\theta)|1\rangle\langle 1| \otimes \mathbb{1} + \theta\mathbb{1} \otimes |1\rangle\langle 1| =: h^{\theta}_{i,i+1}\end{aligned}$$

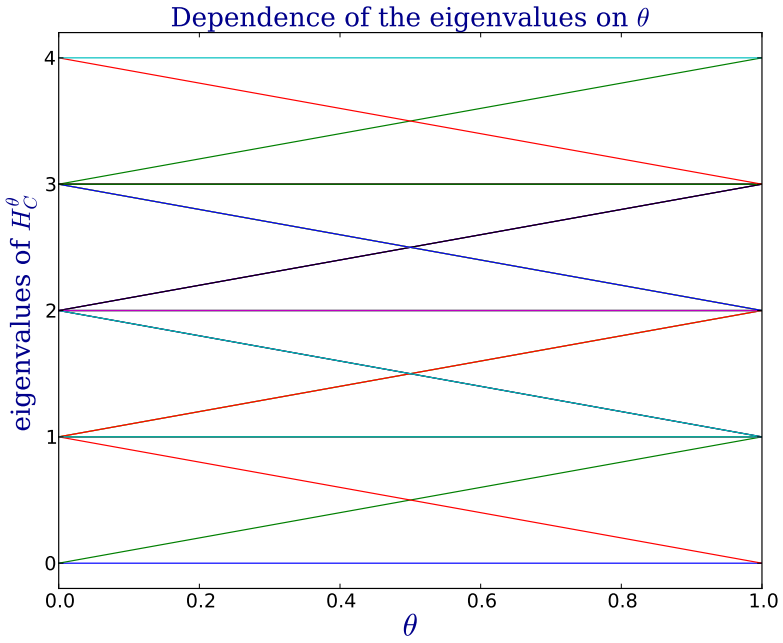

Figure 4.9: The plot depicts the eigenvalues of $H^{\theta}_C := \sum_{i=1}^{L-1} h^{\theta}_{i,i+1} = (1-\theta)|1\rangle\langle 1|_1 + \sum_{i=2}^{L-1}|1\rangle\langle 1|_i + \theta|1\rangle\langle 1|_L$ dependent on θ for a chain of length $L = 5$. For $\theta = 0$ or $\theta = 1$, the ground state energy is degenerate. In the case $\theta = 0$, the ground state space is spanned by $|0\ldots 0\rangle$ and $|0\ldots 01\rangle$, whereas in the case $\theta = 1$, it is generated by $|0\ldots 0\rangle$ and $|10\ldots 0\rangle$. For $\theta \in (0, 1)$, the only ground state is $|0\ldots 0\rangle$.

On a chain of length L, the Hamiltonian is then given by

$$H^{\theta}_C := \sum_{i=1}^{L-1} h^{\theta}_{i,i+1} = (1-\theta)|1\rangle\langle 1|_1 + \sum_{i=2}^{L-1}|1\rangle\langle 1|_i + \theta|1\rangle\langle 1|_L.$$

Interpolating θ from 0 to 1, we see that in the cases $\theta = 0$ or $\theta = 1$ the particle binds to the right or to the left edge. As can also be seen in Fig. 4.9, for $\theta \in (0, 1)$ the degeneracy vanishes, and the particle on the chain does not belong to the ground state (the only ground state is $|0\ldots 0\rangle$). Moreover, the important change only happens at the boundaries. For $\theta \in (0, 1)$, this

Hamiltonian also belongs to the case $n = 0, d = 2$ since there are $d = 2$ possibilities for each site (particle or vacuum), but in the ground state only the vacuum occurs, i.e. $n = 0$ particles appear in the ground state space.

Using a ring of length L instead of the chain, we obtain the Hamiltonian

$$H_R^\theta = \sum_{i=1}^{L} h_{i,i+1}^\theta = \sum_{i=1}^{L} |1\rangle\langle 1|_i,$$

which has no edges at all, meaning that all sites are equivalent. Therefore, the only ground state is given by $|0\dots 0\rangle$, independent of θ.

So, in the case of periodic boundary conditions, the Hamiltonian is constant and there is only one phase for all θ. Using open boundary conditions instead, we can move the particle from one edge to the other. Nevertheless, since the system only changes at the boundaries, we may not call it a phase transition.

Now we strive to investigate whether we obtain an analogous Hamiltonian in the case $d = 3$, $n = 2$. For that, we superpose the Hamiltonian h for (λ_1, λ_2) and the Hamiltonian h for $(\lambda_1^{-1}, \lambda_2^{-1})$, and take the limits $\lambda_1 \to 0$ and $\lambda_2 \to 0$:

$$\begin{aligned}
&\lim_{\substack{\lambda_1\to 0\\ \lambda_2\to 0}} \left[\theta h(\lambda_1,\lambda_2) + (1-\theta) h(\lambda_1^{-1},\lambda_2^{-1})\right] \\
&= \lim_{\substack{\lambda_1\to 0\\ \lambda_2\to 0}} \Bigg[|11\rangle\langle 11| + |22\rangle\langle 22| + \theta\Bigg(\frac{1}{1+\lambda_1^2}\left(|01\rangle - \lambda_1|10\rangle\right)\left(\langle 01| - \lambda_1\langle 10|\right) \\
&+ \frac{1}{1+\lambda_2^2}\left(|02\rangle - \lambda_2|20\rangle\right)\left(\langle 02| - \lambda_2\langle 20|\right) + \frac{1}{1+\alpha^2}\left(\alpha|12\rangle - |21\rangle\right)\left(\alpha\langle 12| - \langle 21|\right)\Bigg) \\
&+ (1-\theta)\Bigg(\frac{1}{1+\lambda_1^2}\left(\lambda_1|01\rangle - |10\rangle\right)\left(\lambda_1\langle 01| - \langle 10|\right) \\
&+ \frac{1}{1+\lambda_2^2}\left(\lambda_2|02\rangle - |20\rangle\right)\left(\lambda_2\langle 02| - \langle 20|\right) + \frac{1}{1+\alpha^2}\left(|12\rangle - \alpha|21\rangle\right)\left(\langle 12| - \alpha\langle 21|\right)\Bigg)\Bigg] \qquad (4.63) \\
&= \theta\left(|11\rangle\langle 11| + |22\rangle\langle 22| + |01\rangle\langle 01| + |02\rangle\langle 02| + \frac{1}{1+\alpha^2}\left(\alpha|12\rangle - |21\rangle\right)\left(\alpha|12\rangle - |21\rangle\right)\right) \\
&+ (1-\theta)\left(|11\rangle\langle 11| + |22\rangle\langle 22| + |10\rangle\langle 10| + |20\rangle\langle 20| + \frac{1}{1+\alpha^2}\left(|12\rangle - \alpha|21\rangle\right)\left(\langle 12| - \alpha\langle 21|\right)\right) \qquad (4.64)
\end{aligned}$$

For $\alpha = 1$, Eq. (4.64) can be simplified, but it is not of the same form as in the case $d = 2$, since there is still a two-particle interaction:

$$\begin{aligned}
&\lim_{\substack{\lambda_1\to 0\\ \lambda_2\to 0}} \left[\theta h(\lambda_1,\lambda_2) + (1-\theta) h(\lambda_1^{-1},\lambda_2^{-2})\right] \\
&= \theta\left(\mathbb{1}\otimes|1\rangle\langle 1| + \mathbb{1}\otimes|2\rangle\langle 2|\right) + (1-\theta)\left(|1\rangle\langle 1|\otimes\mathbb{1} + |2\rangle\langle 2|\otimes\mathbb{1}\right) - \frac{1}{2}\left(|12\rangle + |21\rangle\right)\left(\langle 12| + \langle 21|\right)
\end{aligned}$$

Nevertheless, putting this Hamiltonian on a chain of length L yields

$$\begin{aligned}
H_C := &(1-\theta)\left(|1\rangle\langle 1|_1 + |2\rangle\langle 2|_1\right) + \sum_{i=2}^{L-1}\left(|1\rangle\langle 1|_i + |2\rangle\langle 2|_i\right) + \theta\left(|1\rangle\langle 1|_L + |2\rangle\langle 2|_L\right) \\
&- \frac{1}{2}\sum_{i=1}^{L-1}\left(\left(|12\rangle + |21\rangle\right)\left(\langle 12| + |21\rangle\right)\right)_{i,i+1},
\end{aligned}$$

which is for $\theta = 0$ or $\theta = 1$ the Hamiltonian describing the particles linked to the edges, and for $\theta \in (0, 1)$ the Hamiltonian belonging to $n = 0$ and $d = 3$. Hence, it is indeed possible to move the particles from one edge to the other by scaling θ.

In the case of a ring, all sites become equivalent, and thus the problem again provides translational invariance and resembles periodic boundary conditions as in the case $d = 2$:

$$H_R := \sum_{i=1}^{L} \left(|1\rangle\langle 1|_i + |2\rangle\langle 2|_i - \frac{1}{2} \left((|12\rangle + |21\rangle) \left(\langle 12| + \langle 21| \right) \right)_{i,i+1} \right),$$

where site $L + 1$ is equal to site 1.

All in all, each of the manipulations under consideration was capable of changing the ground state degeneracy without actually causing a phase transition. This fact exhibits the necessity to aim for a finer definition of quantum phase transitions in the case of open boundary conditions for one-dimensional gapped phases.

5 Renormalization Group Transformation

The aim we pursue in this chapter is to understand the long-distance information of PVBS and what $\lambda \to 0$ means in this context. For this, we make use of the Renormalization Group (RG) transformation, explained in section 2.1.1. We examine whether the system is stable under blocking, i.e. grouping adjacent sites into effective new sites. If it is not, we look for physical reasons which may cause these instabilities.

5.1 One Particle Type

First, we examine the case of one particle type that is $n = 1$ and dimension $d = 2$ and see whether the system is stable under blocking sites. Squaring the transfer matrix defined by

$$T = \sum_i v_i \otimes \bar{v}_i, \tag{5.1}$$

we obtain, by using the commutation relations (3.1) and (3.2), that T^2 is of the same form as T:

$$\begin{aligned} T^2 &= (v_0 \otimes \bar{v}_0 + v_1 \otimes \bar{v}_1)(v_0 \otimes \bar{v}_0 + v_1 \otimes \bar{v}_1) \\ &= v_0^2 \otimes \bar{v}_0^2 + v_0 v_1 \otimes \bar{v}_0 \bar{v}_1 + \underbrace{v_1 v_0}_{e^{i\vartheta_{10}}\lambda_1 v_0 v_1} \otimes \underbrace{\bar{v}_1 \bar{v}_0}_{e^{-i\vartheta_{10}}\bar{\lambda}_1 \bar{v}_0 \bar{v}_1} + \underbrace{v_1 v_1}_{0} \otimes \bar{v}_1 \bar{v}_1 \\ &= v_0^2 \otimes \bar{v}_0^2 + \left(\sqrt{1+\lambda_1^2} v_0 v_1\right) \otimes \left(\sqrt{1+\lambda_1^2} \bar{v}_0 \bar{v}_1\right) \end{aligned}$$

Using the definitions

$$v_0' := v_0^2, \qquad v_1' := \sqrt{1+\lambda_1} v_0 v_1, \tag{5.2}$$

T^2 can be recast as

$$T^2 = v_0' \otimes \bar{v}_0' + v_1' \otimes \bar{v}_1',$$

consisting of two terms. That is reasonable as squaring the transfer matrix physically corresponds to grouping two adjacent sites. So two neighboring sites become a new site, and since there are two possibilities for such a blocked site, the transfer matrix squared consists of two summands. These two possibilities for a blocked site are: Either there is one particle on one of the former two sites, or there is no particle on one of the former two sites. Investigating whether the new $v_i', i \in \{0,1\}$ satisfy the commutation relations (3.1) and (3.2)

$$v_1' v_0' = \sqrt{1+\lambda_1^2} v_0 \underbrace{v_1 v_0 v_0}_{e^{i\vartheta_{10}}\lambda_1 v_0 v_1 v_0} = e^{2i\vartheta_{10}} \lambda_1^2 \underbrace{v_0 v_0}_{v_0'} \underbrace{\sqrt{1+\lambda_1^2} v_0 v_1}_{v_1'} \stackrel{!}{=} e^{i\vartheta_{10}'} \lambda_1' v_0' v_1' \tag{5.3}$$

$$v_1' v_1' = \left(1+\lambda_1^2\right) v_0 v_1 v_0 v_1 = \left(1+\lambda_1^2\right) e^{i\vartheta_{10}} \lambda_1 v_0 v_0 \underbrace{v_1 v_1}_{0} = 0 \tag{5.4}$$

leads to the conditions for the new parameters

$$\vartheta_{10}' = 2\vartheta_{10}\,, \qquad \lambda_1' = \lambda_1^2. \tag{5.5}$$

This system, consisting of a chain with one particle type, is stable under blocking.

Applying the commutation relations (5.3) and (5.4) to T^p which corresponds to grouping p sites with $2 \leq p \in \mathbb{N}$ results in

$$T^p = (v_0 \otimes \bar{v}_0 + v_1 \otimes \bar{v}_1)^p = v_0^p \otimes \bar{v}_0^p + \sum_{n=0}^{p-1} \lambda_1^{2n} v_0^{p-1} v_1 \otimes \bar{v}_0^{p-1} \bar{v}_1.$$

Here, the sum can be reduced to two terms as well, leading to new $v_i^{(p)}$s for the p-times blocked sites:

$$v_0^{(p)} := v_0^p \qquad v_1^{(p)} := \sqrt{\sum_{n=0}^{p-1} \lambda_1^{2n}}\, v_0^{p-1} v_1$$

These $v_i^{(p)}$ also satisfy the commutation relations

$$\begin{aligned}
v_1^{(p)} v_1^{(p)} &= \sum_{n=0}^{p-1} \lambda_1^{2n} v_0^{p-1} v_1 v_0^{p-1} v_1 = \sum_{n=0}^{p-1} \lambda_1^{2n} v_0^{p-1} e^{i(p-1)\vartheta_{10}} \lambda_1^{p-1} v_0^{p-1} \underbrace{v_1 v_1}_{0} = 0 \\
v_1^{(p)} v_0^{(p)} &= \sqrt{\sum_{n=0}^{p-1} \lambda_1^{2n}}\, v_0^{p-1} v_1 v_0^p = \sqrt{\sum_{n=0}^{p-1} \lambda_1^{2n}}\, v_0^{p-1} e^{ip\vartheta_{10}} \lambda_1^p v_0^p v_1 \\
&= e^{ip\vartheta_{10}} \lambda_1^p v_0^{(p)} v_1^{(p)} \stackrel{!}{=} e^{i\vartheta_{10}^{(p)}} \lambda_1^{(p)} v_0^{(p)} v_1^{(p)}
\end{aligned}$$

if $\vartheta_{10}^{(p)}$ and $\lambda_1^{(p)}$ fulfill the conditions

$$\vartheta_{10}^{(p)} = p\vartheta_{10}\,, \qquad \lambda_1^{(p)} = \lambda_1^p. \tag{5.6}$$

The relation (5.6) for $\lambda_1^{(p)}$ means that if the number of grouped sites $p \to \infty$, $\lambda_1^{(p)} \to 0$ for $\lambda_1 < 1$ or $\lambda_1^{(p)} \to \infty$ for $\lambda_1 > 1$. We can comprehend what physically happens as follows: For a chain of sufficient length, the particle is located near the boundaries, even if the corresponding λ_1 is close to one. By increasing the value of p, the sites grow ever larger such that the particle gets eventually placed on one of the boundary sites since the probability for the particle to stay far away from the edges decreases rapidly (cf. Eq. (4.6)). Therefore, it is reasonable that the remaining information only consists of the preferred side being either left ($\lambda_1 < 1$) or right ($\lambda_1 > 1$). Since the information how strong the particle binds to the edges seems to be a short-distance information, it vanishes in this limit. So the long-distance information is which boundary a particle binds to. Considering $\lambda_1 < 1$, blocking leads to the limit we investigated in chapter 4.

However, if the chain length L is finite, the actual limit stops at $p = L$ where the entire chain is only one site. In that case, the only information left is whether a particle occurs in the ground state or not which makes it effectively the long-distance information.

5.2 Two Particle Types

Let us now have a look at the case of two particle types, and investigate which effects can be observed by blocking. Squaring T and applying the commutation relations (3.1) and (3.2) yields

$$T^2 = (v_0 \otimes \bar{v}_0 + v_1 \otimes \bar{v}_1 + v_2 \otimes \bar{v}_2)^2 \tag{5.7}$$

$$= v_0^2 \otimes \bar{v}_0^2 + v_0 v_1 \otimes \bar{v}_0 \bar{v}_1 + \underbrace{v_1 v_0 \otimes \bar{v}_1 \bar{v}_0}_{\lambda_1^2 v_0 v_1 \otimes \bar{v}_0 \bar{v}_1} + v_0 v_2 \otimes \bar{v}_0 \bar{v}_2 + \underbrace{v_2 v_0 \otimes \bar{v}_2 \bar{v}_0}_{\lambda_2^2 v_0 v_2 \otimes \bar{v}_0 \bar{v}_2} + v_1 v_2 \otimes \bar{v}_1 \bar{v}_2 + \underbrace{v_2 v_1 \otimes \bar{v}_2 \bar{v}_1}_{\lambda_2^2 \lambda_1^{-2} v_1 v_2 \otimes \bar{v}_1 \bar{v}_2} \tag{5.8}$$

$$= v_0^2 \otimes \bar{v}_0^2 + \left(\lambda_1^2 + 1\right) v_0 v_1 \otimes \bar{v}_0 \bar{v}_1 + \left(\lambda_2^2 + 1\right) v_0 v_2 \otimes \bar{v}_0 \bar{v}_2 + \left(\lambda_2^2 \lambda_1^{-2} + 1\right) v_1 v_2 \otimes \bar{v}_1 \bar{v}_2, \tag{5.9}$$

which is a transfer matrix consisting of four terms, instead of three terms that would have been the structure of T. This is, as previously mentioned in section 2.1.1, because of the four possibilities of states that a blocked site can attain: Grouping two adjacent sites yields for a new site to be occupied by a particle of type 1, by a particle of type 2, by particles of both types or the vacuum. A calculation of the Kraus rank of T^2 yields that T^2 indeed has this structure of four terms. Hence, it is not just physically reasonable but also mathematically consistent. Therefore, the system of a chain with two particle types is not stable under blocking the sites in the first step. Nevertheless, we can also define new matrices $v_i', \quad i \in \{0, 1, 2, (12)\}$ where (12) denotes the new case of two particles of different types being on a site:

$$v_0' := v_0^2, \qquad v_1' := \sqrt{1 + \lambda_1^2}\, v_0 v_1,$$
$$v_2' := \sqrt{1 + \lambda_2^2}\, v_0 v_2, \qquad v_{(12)}' := \sqrt{1 + \lambda_1^{-2}\lambda_2^2}\, v_1 v_2.$$

This will prove useful when developing our new model later on.

We find the following commutation relations that slightly differ from those mentioned in Eq. (3.1) and (3.2) for the new v_i':

$$v_1' v_0' = \sqrt{1 + \lambda_1^2}\, v_0 v_1 v_0 v_0 = e^{2i\vartheta_{10}} \lambda_1^2 \sqrt{1 + \lambda_1^2}\, v_0 v_0 v_0 v_1 = e^{2i\vartheta_{10}} \lambda_1^2 v_0' v_1' \overset{!}{=} e^{i\vartheta_{10}'} \lambda_1' v_0' v_1' \tag{5.10}$$

$$v_2' v_0' = \sqrt{1 + \lambda_2^2}\, v_0 v_2 v_0 v_0 = e^{2i\vartheta_{20}} \lambda_2^2 \sqrt{1 + \lambda_2^2}\, v_0 v_0 v_0 v_2 = e^{2i\vartheta_{20}} \lambda_2^2 v_0' v_2' \overset{!}{=} e^{i\vartheta_{20}'} \lambda_2' v_0' v_2' \tag{5.11}$$

$$v_1' v_2' = \sqrt{1 + \lambda_1^2}\sqrt{1 + \lambda_2^2}\, v_0 v_1 v_0 v_2 = e^{i(\vartheta_{10} + \vartheta_{12} - \vartheta_{20})} \lambda_1^2 \lambda_2^{-2} v_2' v_1' \overset{!}{=} e^{i\vartheta_{12}'} \lambda_1' \lambda_2'^{-1} v_2' v_1' \tag{5.12}$$

$$v_{(12)}' v_0' = \sqrt{1 + \lambda_1^{-2}\lambda_2^2}\, v_1 v_2 v_0 v_0 = e^{2i(\vartheta_{10} + \vartheta_{20})} \lambda_1^2 \lambda_2^2 v_0' v_{(12)}' \overset{!}{=} e^{i\vartheta_{(12)0}'} \lambda_{(12)} v_0' v_{(12)}' \tag{5.13}$$

$$v_1' v_{(12)}' = v_{(12)}' v_1' = v_2' v_{(12)}' = v_{(12)}' v_2' = v_1' v_1' = v_2' v_2' = v_{(12)}' v_{(12)}' = 0 \tag{5.14}$$

The corresponding conditions for the new λ_i' and ϑ_{ij}' are

$$\vartheta_{10}' = 2\vartheta_{10}, \qquad \lambda_1' = \lambda_1^2 \tag{5.15}$$
$$\vartheta_{20}' = 2\vartheta_{20}, \qquad \lambda_2' = \lambda_2^2 \tag{5.16}$$
$$\vartheta_{12}' = \vartheta_{10} + \vartheta_{12} - \vartheta_{20}, \qquad \lambda_1' \lambda_2'^{-1} = \lambda_1^2 \lambda_2^{-2} \tag{5.17}$$
$$\vartheta_{(12)0}' = 2(\vartheta_{10} + \vartheta_{20}), \qquad \lambda_{(12)} = \lambda_1^2 \lambda_2^2. \tag{5.18}$$

Furthermore, there exists an additional commutation relation, which has no analogue among the commutation relations (3.1) and (3.2):

$$v_{(12)}' v_0' = \sqrt{1 + \lambda_1^{-2}\lambda_2^2}\, v_1 v_2 v_0 v_0 = \sqrt{1 + \lambda_1^{-2}\lambda_2^2}\, e^{2i\vartheta_{20}} \lambda_2^2 e^{i\vartheta_{10}} \lambda_1 v_0 v_1 v_0 v_2 \tag{5.19}$$

$$= \frac{\lambda_2^2 \sqrt{\lambda_2^2 + \lambda_1^2}}{\sqrt{1 + \lambda_1^2}\sqrt{1 + \lambda_2^2}} e^{i(\vartheta_{10} + 2\vartheta_{20})} v_1' v_2' \tag{5.20}$$

Taking for granted that these commutation relations are obeyed, we will construct a modified form of PVBS in the next chapter.

6 Blocked PVBS

Investigating the case of two particle types, we learned in section 5.2 that the system showed unstable behavior under blocking. This is not surprising since in the case $n = 2$, T^2 (Eq. (5.9)) consists of four terms as there are four possibilities on two blocked sites: a particle of type 1, a particle of type 2, two particles of both type 1 and type 2, or no particle at all. Due to this, we aim to extend the model of PVBS such that there are four levels per site: $|0\rangle, |1\rangle, |2\rangle, |(12)\rangle$, where (12) denotes the new possibility of both particle types occurring on the same site. Moreover, $v'_{(12)}$ is closely related to the product of v'_1 and v'_2 (cf. Eq. (5.20)) since, depending on how the sites are blocked, two neighboring particles can be on the same site or on two different sites after blocking (see Fig. 6.1). Nevertheless, both possibilities appear in the same superposition state as they did before the blocking, what we have already seen in Eq. (4.27).

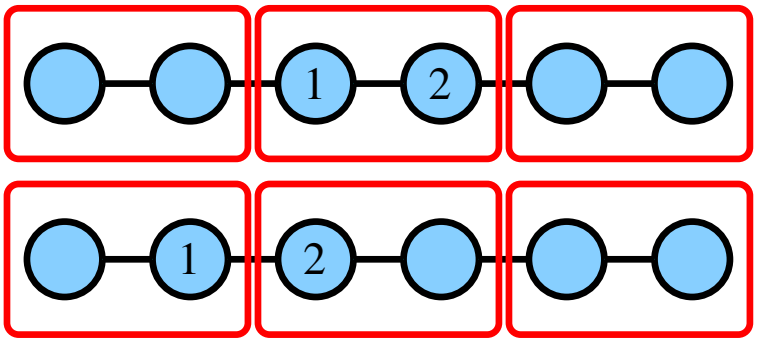

Figure 6.1: The upper image shows two adjacent particles being on the same site after blocking. In contrast, in the lower image, they become located at different but adjacent sites.

Since blocking the sites does not lead to the same structure of the transfer matrix and the commutation relations, we establish a modified form of PVBS, called blocked PVBS, and investigate their properties. The commutation relations that follow from blocking are now assumed as given:

$$v'_j v'_0 = e^{i\vartheta'_{j0}} \lambda'_j v'_0 v'_j, \qquad j = 1, 2 \tag{6.1}$$

$$v'_{(12)} v'_0 = e^{i\vartheta'_{(12)0}} \lambda'_{(12)} v'_0 v'_{(12)}, \qquad \text{where } \lambda'_{(12)} = \lambda'_1 \lambda'_2 \tag{6.2}$$

$$v'_1 v'_2 = e^{i\vartheta'_{12}} \lambda'_1 {\lambda'_2}^{-1} v'_2 v'_1 \tag{6.3}$$

$$v'_{(12)} v'_0 = \lambda'_2 \mu' e^{i(\vartheta_{10}+2\vartheta_{20})} v'_1 v'_2 \qquad \text{where } \mu' = \frac{\sqrt{\lambda'_1 + \lambda'_2}}{\sqrt{1+\lambda'_1}\sqrt{1+\lambda'_2}} \tag{6.4}$$

$$v'_j v'_j = 0, \qquad j = 1, 2, (12) \tag{6.5}$$

$$v'_j v'_{(12)} = v'_{(12)} v'_j = 0, \qquad j = 1, 2 \tag{6.6}$$

6.1 Renormalization Group Transformation

In this section, we check on whether blocked PVBS can be blocked again and still satisfy the new commutation relations, i.e. whether the modified model is stable. Blocking the blocked PVBS and applying the commutation relations (6.1) through (6.6), we obtain the transfer matrix

$$\begin{aligned} T'^2 &= \left(v'_0 \otimes \bar{v}'_0 + v'_1 \otimes \bar{v}'_1 + v'_2 \otimes \bar{v}'_2 + v'_{(12)} \otimes \bar{v}'_{(12)}\right)^2 \\ &= v'^2_0 \otimes \bar{v}'^2_0 + \left(1 + {\lambda'_1}^2\right) v'_0 v'_1 \otimes \bar{v}'_0 \bar{v}'_1 + \left(1 + {\lambda'_2}^2\right) v'_0 v'_2 \otimes \bar{v}'_0 \bar{v}'_2 \\ &+ \left(1 + {\lambda'_1}^{-2} {\lambda'_2}^2 + \frac{{\lambda'_2}^2 (\lambda'_1 + \lambda'_2)(1 + {\lambda'_1}^2 {\lambda'_2}^2)}{(1 + \lambda'_1)(1 + \lambda'_2)}\right) v'_1 v'_2 \otimes \bar{v}'_1 \bar{v}'_2. \end{aligned}$$

As the transfer matrix can be written as a sum of four summands, the structure is retained. Defining new v''_is as

$$\begin{aligned} v''_0 &= v'^2_0, & v''_1 &= \sqrt{1 + \lambda'^2_1}\, v'_0 v'_1 \\ v''_2 &= \sqrt{1 + \lambda'^2_2}\, v'_0 v'_2, & v''_{(12)} &= \underbrace{\sqrt{1 + {\lambda'_1}^{-2} {\lambda'_2}^2 + \frac{{\lambda'_2}^2 (\lambda'_1 + \lambda'_2)(1 + {\lambda'_1}^2 {\lambda'_2}^2)}{(1 + \lambda'_1)(1 + \lambda'_2)}}}_{=: g(\lambda'_1, \lambda'_2)} v'_1 v'_2 \end{aligned}$$

and using the commutation relations (6.1) through (6.6) for the v'_i, the commutation relations for the v''_i

$$\begin{aligned} v''_1 v''_0 &= e^{2i\vartheta'_{10}} \lambda'^2_1 v''_0 v''_1 \stackrel{!}{=} e^{i\vartheta''_{10}} \lambda''_1 v''_0 v''_1 \\ v''_2 v''_0 &= e^{2i\vartheta'_{20}} \lambda'^2_2 v''_0 v''_2 \stackrel{!}{=} e^{i\vartheta''_{20}} \lambda''_2 v''_0 v''_2 \\ v''_1 v''_2 &= e^{i(\vartheta'_{10} + \vartheta'_{12} - \vartheta'_{20})} \lambda'^2_1 \lambda'^{-2}_2 v''_2 v''_1 \stackrel{!}{=} e^{i\vartheta''_{12}} \lambda''_1 \lambda''^{-1}_2 v''_2 v''_1 \\ v''_{(12)} v''_0 &= e^{2i(\vartheta'_{10} + \vartheta'_{20})} \lambda'^2_1 \lambda'^2_2 v''_0 v''_{(12)} \stackrel{!}{=} e^{i\vartheta''_{(12)0}} \lambda''_{(12)} v''_0 v''_{(12)} \\ v''_{(12)} v''_0 &= e^{i(\vartheta'_{10} + 2\vartheta'_{20})} \lambda'_1 \lambda'^2_2 \frac{g(\lambda'_1, \lambda'_2)}{\sqrt{1 + \lambda'^2_1}\sqrt{1 + \lambda'^2_2}} v''_1 v''_2 \\ &= e^{i(\vartheta'_{10} + 2\vartheta'_{20})} \lambda''_2 \underbrace{\frac{\sqrt{\lambda''_1 + \lambda''_2 + \lambda''_1 \lambda''_2 \mu'^2\,(1 + \lambda''_1 \lambda''_2)}}{\sqrt{1 + \lambda''_1}\sqrt{1 + \lambda''_2}}}_{=: \mu''} v''_1 v''_2 \end{aligned}$$

$$v''_1 v''_{(12)} = v''_{(12)} v''_1 = v''_2 v''_{(12)} = v''_{(12)} v''_2 = v''_1 v''_1 = v''_2 v''_2 = v''_{(12)} v''_{(12)} = 0$$

can be verified under the following conditions:

$$\begin{aligned} \vartheta''_{10} &= 2\vartheta'_{10} & \lambda''_1 &= \lambda'^2_1 \\ \vartheta''_{20} &= 2\vartheta'_{20} & \lambda''_2 &= \lambda'^2_2 \\ \vartheta''_{12} &= \vartheta'_{10} + \vartheta'_{12} - \vartheta'_{20} & \lambda''_1 \lambda''^{-1}_2 &= \lambda'^2_1 \lambda'^{-2}_2 \\ \vartheta''_{(12)0} &= 2(\vartheta'_{10} + \vartheta'_{20}) & \lambda''_{(12)} &= \lambda'^2_1 \lambda'^2_2 \end{aligned}$$

Since the commutation relations are satisfied, the system is stable under blocking. Therefore, we can now proceed to study the ground states.

6.2 Investigation of the Ground States

Let us now examine what ground states are provided by the v_i', $i \in \{0, 1, 2, (12)\}$. Making use of the commutation relations (6.1) through (6.6) we found by blocking the sites, the ground states on a chain of length $L = 2$ can be written as follows if we require the ground states again to be given by $\psi(B)$:

$$\psi(B) = \sum_{i_1,i_2\in\{0,1,2,(12)\}} \mathrm{Tr}(Bv'_{i_1}v'_{i_2})|i_2 i_1\rangle \tag{6.7}$$

$$\begin{aligned} &= \mathrm{Tr}(Bv'_0v'_0)|00\rangle + \mathrm{Tr}(Bv'_0v'_1)\left(|10\rangle + e^{i\vartheta'_{10}}\lambda'_1|01\rangle\right) + \mathrm{Tr}(Bv'_0v'_2)\left(|20\rangle + e^{i\vartheta'_{20}}\lambda'_2|02\rangle\right) \\ &+ \mathrm{Tr}(Bv'_0v'_{(12)})\Big(|(12)0\rangle + e^{i\vartheta'_{(12)0}}\lambda'_1\lambda'_2|0(12)\rangle + {\mu'}^{-1}e^{-i(\vartheta_{10}+2\vartheta_{20})}e^{i\vartheta'_{(12)0}}\lambda'_1|21\rangle \\ &+ {\mu'}^{-1}\lambda'_1\alpha^{-1}e^{i\vartheta'_{12}}e^{-i(\vartheta_{10}+2\vartheta_{20})}e^{i\vartheta'_{(12)0}}|12\rangle\Big) \end{aligned} \tag{6.8}$$

The ground state space is four-dimensional what can be proven as follows:

Choose $B = B_0v'_1v'_2$, where $B_0 \in \mathrm{Mat}(\mathbb{C})^{4\times4}$ has to be selected such that $\mathrm{Tr}(B_0v'_1v'_2v'_0v'_0) \neq 0$. Since B consists of v'_1 and v'_2, $\mathrm{Tr}(B_0v'_1v'_2v'_0v'_1) = \mathrm{Tr}(B_0v'_1v'_2v'_0v'_2) = \mathrm{Tr}(B_0v'_1v'_2v'_0v'_{12}) = 0\ \forall B_0 \in \mathrm{Mat}(\mathbb{C})^{4\times4}$ because of Eq. (6.5) and (6.6). Therefore, $|00\rangle$ is linearly independent of the other vectors. Then there is the possibility of choosing $B = B_1v'_2$, where $B_1 \in \mathrm{Mat}(\mathbb{C})^{4\times4}$ must satisfy $\mathrm{Tr}(B_1v'_2v'_0v'_1) \neq 0$. Applying Eq. (6.5) and (6.6) yields $\mathrm{Tr}(B_1v'_2v'_0v'_2) = \mathrm{Tr}(B_1v'_2v'_0v'_{12}) = 0$. If $\mathrm{Tr}(B_1v'_2v'_0v'_0) \neq 0$, we can subtract $|00\rangle$ since we know that it is possible to create $|00\rangle$ linearly independently. Hence, $|10\rangle + e^{i\vartheta'_{10}}\lambda'_1|01\rangle$ can also be chosen linearly independent. But B can be taken such that $B = B_2v'_1$, where $B_2 \in \mathrm{Mat}(\mathbb{C})^{4\times4}$ and $\mathrm{Tr}(B_2v'_1v'_0v'_2) \neq 0$. This leads to $\mathrm{Tr}(B_2v'_1v'_0v'_1) = \mathrm{Tr}(B_2v'_1v'_0v'_{12}) = 0$ by using Eq. (6.5) and (6.6). Again, if $\mathrm{Tr}(B_2v'_1v'_0v'_0) \neq 0$, $|00\rangle$ can be subtracted since $|00\rangle$ is linearly independent of the other vectors. Thus, $|20\rangle + e^{i\vartheta'_{20}}\lambda'_2|02\rangle$ can be chosen linearly independent. So, the fourth vector is linearly independent of the other three vectors, and the ground state space is four-dimensional.

6.3 Construction of the Parent Hamiltonian

Now, we construct the parent Hamiltonian of the ground states that we have just calculated. The parent Hamiltonian is given by the projector onto the orthogonal complement of the ground state space according to section 2.2:

$$h = \Pi_{\psi_\perp} = \mathbb{1} - \Pi_{\psi(B)}, \tag{6.9}$$

where $\Pi_{\psi(B)}$ is the projector onto the ground state space. An orthonormal basis of the ground state space which was calculated in Eq. (6.8) is given by

$$|\varphi_1\rangle := |00\rangle \tag{6.10}$$

$$|\varphi_2\rangle := \frac{1}{\sqrt{1+\lambda_1'^2}}\left(|10\rangle + e^{i\vartheta'_{10}}\lambda'_1|01\rangle\right) \tag{6.11}$$

$$|\varphi_3\rangle := \frac{1}{\sqrt{1+\lambda_2'^2}}\left(|20\rangle + e^{i\vartheta'_{20}}\lambda'_2|02\rangle\right) \tag{6.12}$$

$$\begin{aligned} |\varphi_4\rangle := \frac{1}{\sqrt{1+\lambda_1'^2\lambda_2'^2+\mu'^{-2}\lambda_1'^2+\mu'^{-2}\lambda_2'^2}}&\Big(|(12)0\rangle + e^{i\vartheta'_{(12)0}}\lambda'_1\lambda'_2|0(12)\rangle \\ &+ {\mu'}^{-1}e^{-i(\vartheta_{10}+2\vartheta_{20})}e^{i\vartheta'_{(12)0}}\lambda'_1\left(|21\rangle + \alpha^{-1}e^{i\vartheta'_{12}}|12\rangle\right)\Big). \end{aligned} \tag{6.13}$$

Therefore, the Hamiltonian can be written as

$$
\begin{aligned}
h &= \mathbb{1} - |\varphi_1\rangle\langle\varphi_1| - |\varphi_2\rangle\langle\varphi_2| - |\varphi_3\rangle\langle\varphi_3| - |\varphi_4\rangle\langle\varphi_4| && (6.14)\\
&= |(12)1\rangle\langle(12)1| + |1(12)\rangle\langle 1(12)| + |(12)2\rangle\langle(12)2| + |2(12)\rangle\langle 2(12)| + |11\rangle\langle 11| + |22\rangle\langle 22|\\
&+ |01\rangle\langle 01| + |10\rangle\langle 10| - \frac{1}{1+\lambda_1'^2}\left(|10\rangle + e^{i\vartheta'_{10}}\lambda_1'|01\rangle\right)\left(\langle 10| + e^{-i\vartheta'_{10}}\lambda_1'\langle 10|\right)\\
&+ |02\rangle\langle 02| + |20\rangle\langle 20| - \frac{1}{1+\lambda_2'^2}\left(|20\rangle + e^{i\vartheta'_{20}}\lambda_2'|02\rangle\right)\left(\langle 20| + e^{-i\vartheta'_{20}}\lambda_2'\langle 20|\right)\\
&+ |(12)(12)\rangle\langle(12)(12)| + |(12)0\rangle\langle(12)0| + |0(12)\rangle\langle 0(12)| + |12\rangle\langle 12| + |21\rangle\langle 21| - |\varphi_4\rangle\langle\varphi_4| && (6.15)\\
&= |(12)1\rangle\langle(12)1| + |1(12)\rangle\langle 1(12)| + |(12)2\rangle\langle(12)2| + |2(12)\rangle\langle 2(12)| + |11\rangle\langle 11| + |22\rangle\langle 22|\\
&+ \frac{1}{1+\lambda_1'^2}\left(|01\rangle - e^{-i\vartheta'_{10}}\lambda_1'|10\rangle\right)\left(\langle 01| - e^{i\vartheta'_{10}}\lambda_1'\langle 10|\right)\\
&+ \frac{1}{1+\lambda_2'^2}\left(|02\rangle - e^{-i\vartheta'_{20}}\lambda_2'|20\rangle\right)\left(\langle 02| - e^{i\vartheta'_{20}}\lambda_2'\langle 20|\right) + |(12)(12)\rangle\langle(12)(12)|\\
&+ \underbrace{|(12)0\rangle\langle(12)0| + |0(12)\rangle\langle 0(12)| + |12\rangle\langle 12| + |21\rangle\langle 21| - |\varphi_4\rangle\langle\varphi_4|}_{=:\mathcal{A}} && (6.16)
\end{aligned}
$$

Since $|(12)0\rangle\langle(12)0|+|0(12)\rangle\langle 0(12)|+|12\rangle\langle 12|+|21\rangle\langle 21|$ is the unity operator on the subspace $\mathcal{S} := \text{span}\{\ |12\rangle, |21\rangle, |(12)0\rangle, |0(12)\rangle\}$, $\mathcal{A}$ defined in Eq. (6.16) is the projector onto the orthogonal complement of $|\varphi_4\rangle$. We search for a way to write $\mathcal{A}$ in in the form $\mathcal{A} = |\varphi_\perp^{(1)}\rangle\langle\varphi_\perp^{(1)}|+|\varphi_\perp^{(2)}\rangle\langle\varphi_\perp^{(2)}|+|\varphi_\perp^{(3)}\rangle\langle\varphi_\perp^{(3)}|$ where $\{|\varphi_\perp^{(i)}\rangle,\ i=1,2,3\}$ is a orthonormal basis of the orthogonal complement of $|\varphi_4\rangle$. For that, we have to find an orthonormal set of three vectors $\left(|\varphi_\perp^{(1)}\rangle, |\varphi_\perp^{(2)}\rangle, \text{and } |\varphi_\perp^{(3)}\rangle\right)$ lying in the subspace $\mathcal{S}$ that are required to be perpendicular to $|\varphi_4\rangle$. For that, they have to satisfy the conditions

$$\langle\varphi_4|\varphi_\perp^{(1)}\rangle = 0, \tag{6.17}$$
$$\langle\varphi_4|\varphi_\perp^{(2)}\rangle = 0, \tag{6.18}$$
$$\langle\varphi_4|\varphi_\perp^{(3)}\rangle = 0, \tag{6.19}$$
$$\langle\varphi_\perp^{(1)}|\varphi_\perp^{(2)}\rangle = 0, \tag{6.20}$$
$$\langle\varphi_\perp^{(1)}|\varphi_\perp^{(3)}\rangle = 0, \tag{6.21}$$
$$\langle\varphi_\perp^{(2)}|\varphi_\perp^{(3)}\rangle = 0. \tag{6.22}$$

As $|\varphi_\perp^{(i)}\rangle$ for $i \in \{1,2,3\}$ should be of the form

$$|\varphi_\perp^{(i)}\rangle = \beta_i|(12)0\rangle + \kappa_i|0(12)\rangle + \eta_i|12\rangle + \zeta_i|21\rangle,$$

where $\beta_i, \kappa_i, \eta_i, \zeta_i \in \mathbb{C}$, there are 12 independent constants but only 9 conditions (6 from Eq. (6.17) through (6.22) + 3 for normalizations of $|\varphi_\perp^{(i)}\rangle$). Therefore, we have 3 independent constants free, and we choose $\zeta_1 = \eta_1 = \kappa_2 = 0$. Conditions (6.17) through (6.19) yield for $i \in \{1,2,3\}$

$$\beta_i + e^{-i\vartheta'_{(12)0}}\lambda_1'\lambda_2'\kappa_i + e^{i(\vartheta_{10}+2\vartheta_{20})}e^{-i\vartheta'_{(12)0}}\lambda_1'\mu'^{-1}\zeta_i + e^{-i\vartheta'_{12}}e^{i(\vartheta_{10}+2\vartheta_{20})}e^{-i\vartheta'_{(12)0}}\lambda_2'\mu'^{-1}\eta_i = 0 \tag{6.23}$$

$$\Rightarrow \beta_i = -e^{-i\vartheta'_{(12)0}}\left(\lambda_1'\lambda_2'\kappa_i + e^{i(\vartheta_{10}+2\vartheta_{20})}\mu'^{-1}\lambda_1'\zeta_i + e^{-i\vartheta'_{12}}e^{i(\vartheta_{10}+2\vartheta_{20})}\mu'^{-1}\lambda_2'\eta_i\right). \tag{6.24}$$

Applying $\zeta_1 = \eta_1 = 0$, we obtain

$$\beta_1 = -e^{-i\vartheta'_{(12)0}}\lambda_1'\lambda_2'\kappa_1 \tag{6.25}$$

and therefore

$$|\varphi_\perp^{(1)}\rangle = \kappa_1 \left(|0(12)\rangle - e^{-i\vartheta'_{(12)0}}\lambda'_1\lambda'_2|(12)0\rangle\right), \tag{6.26}$$

where κ_1 is used for normalization. Conditions (6.20) through (6.22) lead to

$$\bar{\beta}_i\beta_j + \bar{\kappa}_i\kappa_j + \bar{\zeta}_i\zeta_j + \bar{\eta}_i\eta_j \stackrel{!}{=} 0 \qquad \forall i \neq j \in \{1,2,3\} \tag{6.27}$$

and then substituting Eq. (6.24) and $\kappa_2 = 0$ into Eq. (6.27) for $i = 1$ and $j = 2$ leads to

$$\lambda_1'^2\lambda'_2\bar{\kappa}_1 e^{i(\vartheta_{10}+2\vartheta_{20})}\mu'^{-1}\left(\zeta_2 + e^{-i\vartheta'_{12}}\alpha^{-1}\eta_2\right) = 0 \tag{6.28}$$

$$\Rightarrow \zeta_2 = -e^{-i\vartheta'_{12}}\alpha^{-1}\eta_2 \tag{6.29}$$

$$\Rightarrow \beta_2 = 0 \tag{6.30}$$

$$\Rightarrow |\varphi_\perp^{(2)}\rangle = \eta_2\left(|12\rangle - e^{-i\vartheta'_{12}}\alpha^{-1}|21\rangle\right), \tag{6.31}$$

where η_2 is used for normalization. From condition (6.21) follows

$$\kappa_3 = e^{i\vartheta'_{(12)0}}\lambda'_1\lambda'_2\beta_3 \tag{6.32}$$

and condition (6.22) gives

$$\eta_3 = e^{i\vartheta'_{12}}\alpha^{-1}\zeta_3. \tag{6.33}$$

Inserting Eq. (6.32) and (6.33) into Eq. (6.24) yields

$$\beta_3 = -e^{-i\vartheta'_{(12)0}}\left(e^{i\vartheta'_{(12)0}}\lambda_1'^2\lambda_2'^2\beta_3 + e^{i(\vartheta_{10}+2\vartheta_{20})}\mu'^{-1}\lambda'_1\zeta_3\left(1+\alpha^{-2}\right)\right) \tag{6.34}$$

$$\Rightarrow \beta_3 = \frac{-e^{i(\vartheta_{10}+2\vartheta_{20})}e^{-i\vartheta'_{(12)0}}\mu'^{-1}\lambda'_1\left(1+\alpha^{-2}\right)}{1+\lambda_1'^2\lambda_2'^2}\zeta_3 \tag{6.35}$$

$$\Rightarrow |\varphi_\perp^{(3)}\rangle = \zeta_3\left(\frac{-e^{i(\vartheta_{10}+2\vartheta_{20})}e^{-i\vartheta'_{(12)0}}\lambda'_1\left(1+\alpha^{-2}\right)}{\left(1+\lambda_1'^2\lambda_2'^2\right)\mu'}\left(|(12)0\rangle + e^{i\vartheta'_{(12)0}}\lambda'_1\lambda'_2|0(12)\rangle\right) + |21\rangle + e^{i\vartheta'_{12}}\alpha^{-1}|12\rangle\right) \tag{6.36}$$

where ζ_3 is used for normalization.

Substituting $\mathcal{A}$ with $|\varphi_\perp^{(1)}\rangle\langle\varphi_\perp^{(1)}| + |\varphi_\perp^{(2)}\rangle\langle\varphi_\perp^{(2)}| + |\varphi_\perp^{(3)}\rangle\langle\varphi_\perp^{(3)}|$ in Eq. (6.16) leads to the Hamiltonian

$$\begin{aligned} h = {} & |\varphi_\perp^{(1)}\rangle\langle\varphi_\perp^{(1)}| + |\varphi_\perp^{(2)}\rangle\langle\varphi_\perp^{(2)}| + |\varphi_\perp^{(3)}\rangle\langle\varphi_\perp^{(3)}| + |11\rangle\langle 11| + |22\rangle\langle 22| \\ & + \frac{1}{1+\lambda_1'^2}\left(|01\rangle - e^{-i\vartheta'_{10}}\lambda'_1|10\rangle\right)\left(\langle 01| - e^{i\vartheta'_{10}}\lambda'_1\langle 10|\right) \\ & + \frac{1}{1+\lambda_2'^2}\left(|02\rangle - e^{-i\vartheta'_{20}}\lambda'_2|20\rangle\right)\left(\langle 02| - e^{i\vartheta'_{20}}\lambda'_2\langle 20|\right) \\ & + |(12)1\rangle\langle(12)1| + |1(12)\rangle\langle 1(12)| + |(12)2\rangle\langle(12)2| + |2(12)\rangle\langle 2(12)| + |(12)(12)\rangle\langle(12)(12)|. \end{aligned} \tag{6.37}$$

The desired ground states (6.10) through (6.13) are ground states of this Hamiltonian by construction. These are also the only ground states since $\{|\varphi_\perp^{(1)}\rangle, |\varphi_\perp^{(2)}\rangle, |\varphi_\perp^{(3)}\rangle, |\varphi_4\rangle\} =: \mathcal{B}$ is a orthonormal basis of $\mathrm{span}\{|0(12)\rangle, |(12)0\rangle, |12\rangle, |21\rangle\} =: \mathbb{B}$ by construction, and $\mathcal{B}$ (and thus $\mathbb{B}$) is mapped onto the subspace $\mathrm{span}\{|\varphi_\perp^{(1)}\rangle, |\varphi_\perp^{(2)}\rangle, |\varphi_\perp^{(3)}\rangle\}$. Therefore, the image of h restricted to $\mathbb{B}$ is three-dimensional and the kernel has dimension one. Restricted to the two-dimensional subspaces $\mathrm{span}\{|10\rangle, |01\rangle\}$ and $\mathrm{span}\{|20\rangle, |02\rangle\}$, respectively, the dimension of the kernel of h is one in each case. In the remaining subspace, h is diagonal and it is obvious that $|00\rangle$ is the only eigenvector corresponding to eigenvalue zero.

6.4 Limits $\lambda_i' \to 0$

Having determined a basis of ground states, we now take the limits of strong bindings $\lambda_1' \to 0$, $\lambda_2' \to 0$ where $\alpha = \text{const.}$ of Eq. (6.8) to study the behavior of the gap in this new model. Taking the limits yields the possible ground states

$$\psi_{\lambda_1',\lambda_2'=0}(B) = \mathrm{Tr}(Bv_0'v_0')|00\rangle + \mathrm{Tr}(Bv_0'v_1')|10\rangle + \mathrm{Tr}(Bv_0'v_2')|20\rangle + \mathrm{Tr}(Bv_0'v_{12}')|(12)0\rangle. \quad (6.38)$$

These states look reasonable since two particles of different types can be placed on a blocked site, and if both of them want to be as far left as possible, they should be located at the outermost left site.

Finally, taking the limit $\lambda_1' \to 0, \lambda_2' \to 0$ where $\alpha = \text{const.}$ of the Hamiltonian in Eq. (6.37) and using that $\lambda_1'\mu'^{-1} \to 0$ for $\lambda_1' \to 0, \lambda_2' \to 0$ results in

$$\begin{aligned}
\lim_{\substack{\lambda_1'\to 0\\ \lambda_2'\to 0,\alpha=\text{const}}} h &= |0(12)\rangle\langle 0(12)| + \frac{1}{1+\alpha^{-2}}\left(|12\rangle - e^{-i\vartheta_{12}'}\alpha^{-1}|21\rangle\right)\left(\langle 12| - e^{i\vartheta_{12}'}\alpha^{-1}\langle 21|\right) \\
&+ \frac{1}{1+\alpha^{-2}}\left(|21\rangle + e^{i\vartheta_{12}'}\alpha^{-1}|12\rangle\right)\left(\langle 21| + e^{-i\vartheta_{12}'}\alpha^{-1}\langle 12|\right) + |11\rangle\langle 11| + |22\rangle\langle 22| \\
&+ |01\rangle\langle 01| + |02\rangle\langle 02| + |(12)1\rangle\langle (12)1| + |1(12)\rangle\langle 1(12)| \\
&+ |(12)2\rangle\langle (12)2| + |2(12)\rangle\langle 2(12)| + |(12)(12)\rangle\langle (12)(12)| \\
&= \mathbb{1}\otimes|1\rangle\langle 1| + \mathbb{1}\otimes|2\rangle\langle 2| + \mathbb{1}\otimes|(12)\rangle\langle (12)|.
\end{aligned}$$

This is consistent with the ground states we obtained from $\psi(B)$ (Eq. (6.38)) since these ground states are the only ones of this Hamiltonian. So the Hamiltonian acting on a chain where $L > 2$ is given by

$$H = \sum_{i=2}^{L}\left(|1\rangle\langle 1|_i + |2\rangle\langle 2|_i + |(12)\rangle\langle (12)|_i\right).$$

This Hamiltonian does not contain two-particle interactions anymore, and turning on a perturbation on the first site, acting on both particle types individually as well as on the combined state (12),

$$Y := \left(|1\rangle\langle 1| + |2\rangle\langle 2| + |(12)\rangle\langle (12)|\right)\otimes \mathbb{1}_{L-1} \quad (6.39)$$

to the Hamiltonian yields

$$H' := H + Y = \sum_{i=1}^{L}\left(|1\rangle\langle 1|_i + |2\rangle\langle 2|_i + |(12)\rangle\langle (12)|_i\right). \quad (6.40)$$

The only corresponding ground state is obviously $|0\ldots 0\rangle$. Hence, by extending the model with an effective new state, we were able to eventually make it stable under blocking. Moreover, we have found a translation invariant Hamiltonian for the problematic case of two particle types, only by modifying the boundary. So, unlike before, there is no need anymore for a perturbation that removes two-particle interactions by manipulating the entire chain.

Even the modified model of PVBS yields, in the case of a vanishing gap, a change in the ground state degeneracy at the boundary whereas the bulk of the system behaves continuously. Thus, this discontinuity at the edge cannot be called phase transition.

7 Conclusion

In this thesis, we have studied the role of boundaries in the classification of one-dimensional quantum phases and transitions between them. A quantum phase transition is usually referred to as a discontinuous behavior in a physical system as a whole at zero temperature due to a change in some external parameter. A common means to test for quantum phase transitions is to examine the behavior of the gap between the system's ground state energy and the energy of the first excited state. This classification via gap yielded for one-dimensional gapped phases with periodic boundary conditions that there exists only one phase[2, 3]. For open boundary conditions, in contrast, there is a need for finer classifications[4]. Our aim was to test whether the disappearance of a gap implies a discontinuous behavior in the system and thus a phase transition in the case of open boundary conditions. For that, we investigated a specific model, called the PVBS-model.

The PVBS-model is a spin chain consisting of L sites which can be occupied by $d-1$ particle types or the vacuum, and it is based on open boundary conditions. The ground state degeneracy is given by 2^n and n is the number of particles appearing in the ground state space. A special property of these PVBS is that particles bind to the edges. For that, the total Hamiltonian depends on positive parameters $\lambda_i \neq 1$ which describe how strong a particle of type i binds to the boundaries. Specifically, this means that a value less than one denotes a particle binding to the left edge, and a value greater than one corresponds to the right edge.

The examination of PVBS regarding the boundaries and possible phase transitions yielded that in this particular model, the definitions of phase transitions are not totally equivalent. We observed the gap closing which resulted in a change in the ground state degeneracy, but this only led to discontinuities at the boundary. The bulk of the system still behaved continuously; it even remained unchanged.

For the cases of both one and two particle types (corresponding to $d = 2$ and $d = 3$, respectively), we examined the behavior of the system in the limit of strongest binding to the left edge, i.e. $\lambda_i \to 0$. In this way, we were able to simplify both the Hamiltonian and the ground states. This allowed us to find a simple path for the Hamiltonian on which the gap vanished. In particular, the gap's vanishing was induced by considering various perturbations that might correspond to e.g. an external magnetic field. Although each only acted on the left boundary of the system, they were capable of decreasing the ground state degeneracy and thus representing a type of discontinuous behavior. However, since all ground states only differed in their occupancies at the boundary, states leaving the ground state space did not cause the bulk of the system to undergo any changes. Hence, it should by definition not be termed phase transition.

An interesting effect that occurred in the case of one particle type was that, for the right scale of perturbation strength, the Hamiltonian became translation invariant and thus was of the same form as the one with periodic boundary conditions. This convenient property could not be achieved for two particle types owing to certain two-particle interactions in the Hamiltonian. Therefore, we initially tried to eliminate those by a corresponding perturbation. Unfortunately, albeit not causing a phase transition, this perturbation had to act on the entire chain.

Another point of study was to gain knowledge of the long-distance description of PVBS, so we examined a Renormalization Group transformation and the system's behavior under blocking. In this context, blocking means grouping adjacent sites to effective new sites. For one particle type, the system proved stable under blocking, and the long-distance information contained only whether a particle binds to the left or to the right edge, disregarding information on the binding strength. In contrast, the two-particle system turned out to be unstable under blocking insofar as grouping two sites produced four possible states for the new site instead of three, which would have been the stable behavior. Therefore, we developed a new form of PVBS. Here, a site could be occupied by particle type 1, particle type 2, both types, or the vacuum; thus yielding four possibilities. For that system, similar investigations have been done and led to the same result of the need for an extended definition of phase transitions.

Besides, this new form of PVBS was also capable of solving the above mentioned problem in the case of two particle types. So it achieved the desired translational invariance by only taking influence on the boundary and not on the chain as a whole.

So, all in all we can conclude that, for open boundary conditions, the definitions of phase transitions in one dimension are not equivalent. Depending on which definition one refers to, one may say a phase transition of the system has been observed or not. In order to avoid that problem of ambiguity, further positional information should become an essential part of the definition, i.e. whether only the boundary was affected or the bulk of the system changed discontinuously.

For further investigation, it would be an interesting task to analyze the role of boundaries in gapped phases in higher dimensions where boundaries are much more complex.

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Bibliography

[1] S. Bachmann, S. Michalakis, B. Nachtergaele, and R. Sims, *Automorphic Equivalence within Gapped Phases of Quantum Lattice Systems*, Commun. Math. Phys. **309**, 835 (2012), arXiv:1102.0842

[2] N. Schuch, D. Pérez-García, and J. I. Cirac, *Classifying quantum phases using MPS and PEPS*, Phys. Rev. B **84**, 165139 (2011), arXiv:1010.3732v3

[3] X. Chen, Z.-C. Gu, X.-G. Wen, *Classification of Gapped Symmetric Phases in 1D Spin Systems*, Phys. Rev. B **83**, 035107 (2011), arXiv:1008.3745v2

[4] S. Bachmann and B. Nachtergaele, *Product vacua with boundary states*, Phys. Rev. B **86**, 035149 (2012), arXiv:1112.4097v3

[5] R. Orús, *A Practical Introduction to Tensor Networks: Matrix Product States and Projected Entangled Pair States*, Ann. Phys. **349**, 117 (2014), arXiv:1306.2164v2

[6] N. Schuch, *Condensed Matter Applications of Entanglement Theory*, Lecture Notes of the 44$^{\text{th}}$ IFF Spring School, Forschungszentrum Jülich, 2013

[7] F. Verstraete, J. I. Cirac, J. I. Latorre, E. Rico, and M. M. Wolf, *Renormalization group transformations on quantum states*, Phys. Rev. Lett. **94**, 140601 (2005), arXiv:quant-ph/0410227v1

[8] D. Pérez-García, F. Verstraete, M. M. Wolf, and J. I. Cirac, *Matrix Product State Representations*, Quantum Inf. Comput. **7**, 401 (2007), arXiv:quant-ph/0608197v2

[9] S. Bachmann and B. Nachtergaele, *Product vacua with boundary states and the classification of gapped phases*, Commun. Math. Phys. **329**, 509 (2014), arXiv:1212.3718v3