Master thesis

On the study of bound states in quantum lattice models

Presented by

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Abstract

In this master's thesis the properties of multi-(quasi-)particle bound-states in quantum lattice models are studied. We discuss numerical diagonalisation techniques to detect bound-states using the scaling of their average distance on finite systems and to obtain series expansions of bound-state energies. These methods are tested using known results of the one-dimensional XXZ-model and used to study the three-triplon bound states of the antiferromagnetic Heisenberg ladder. We also study analytical methods based on zero-temperature Green's functions and the Dyson equation to reduce the calculation of two-particle bound-state energies in the presence of finite range interactions to a finite matrix problem. This technique is again tested using the established results of the one-dimensional XXZ-model and further used to study the bound-state properties of the two-dimensional XXZ-model on a square lattice. We also use this technique to obtain series expansions of two-triplon bound-state energies of the Heisenberg ladder with additional cross terms. In order to apply this method we introduce an exact mapping between bosonic and hard-core bosonic operators, which does not rely on infinite onsite repulsion. After that we provide an overview over a recursion based technique useful for the calculation of exact solutions of one-dimensional two-particle bound states even in the presents of long-range interactions. We use this ansatz to obtain the known eigenvectors and eigenenergies of the one-dimensional discrete Hydrogen atom and calculate an equation for the eigenenergy of a one-dimensional system with exponentially decaying interactions. In the Appendix of this work we provide results for the three particle bound-state energy of a one-dimensional system of hard-core bosons with a genuine three-particle density-density-density interaction and provide a compact formula for the general n-particle bound-states of the one-dimensional XXZ-model based on a special case of the geometric Bethe ansatz.

Contents

I Introduction

Connections are formed all the time, be it the formation of a friendship between two persons, a trade agreement between countries or two LEGO stones interlocking. The concept of two or more constituents forming a new whole has fascinated physicists ever since, from the scale of the earth being bound to the sun, never moving to far or to close to it, in a stable manner, down to atoms, representing bound states between a nucleus and electrons. This last example is of special interest, as in contrast to the planetary motion, which is well explained by the theories of Newtonian Gravity and General Relativity, the atom fails to be explained by classical electrodynamics, as a negatively charged electron moving around a nucleus in a planet like manner would inevitably radiate away all its energy in the form of electromagnetic radiation. A solution to this problem was found during the inception of quantum mechanics, wherein the electron moving around a nucleus was no longer allowed to assume states of arbitrary energy values and instead was restricted to certain discrete energy states. Since then understanding the formation of bound states has been a focal point in quantum mechanics research, from its roots in the solutions of the hydrogen atom, the combination of neutral atoms to molecules via bonding orbitals, up to the formation of entire solids with atoms bound together in a crystalline structure. In this realm of solid-state systems the peculiar property arises that their low-energy excitations can again be interpreted as so called quasi-particles. These include the dressed electrons near the Fermi surface, the vibrational modes of the atomic lattice, we call phonons and magnetic excitations like magnons. These quasi-particles can interact with one another and form new bound states within the larger bound state that is the solid itself. Some examples of these are bound states between dressed electrons and holes in semiconductors called excitons, which interact via the Coulomb interaction, Cooper pairs, which are described by two dressed electrons, bound via phonon mediated attractive interactions (in conventional superconductors) and magnon-magnon bound-states in spin systems [1] [2], with an interaction between spins originating in the Coulomb interaction of the particles they are part of. The presence of such quasi-particle bound states can alter material properties in unique ways and understanding this menagerie of different binding phenomena is essential for the study of complex phases of matter, providing not only a rich range of physical realisations in solid-state systems, but also a playground for many advanced numerical and analytical techniques necessary to get a hold on these strongly correlated many-particle systems.

Research in this broad field is still active, with this thesis being partially motivated by the study of three-quasi-particle bound-states in spin-ladder systems [3] connected to high temperature superconductivity [4]. This master's thesis will discuss several techniques to study the multi-particle low energy sectors of quantum lattice models using numerical, perturbative and analytical means, with a focus on magnetic systems.
This thesis is structured as followed:
First, we will provide an overview on the general properties of multi-particle spectra and the problems arising when studying them in chapter II.
Next, we will discuss perturbative continuous unitary transformations (pCUT) in section III.1 and linked-cluster expansions in section III.2 as prerequisite techniques to obtain particle number conserving effective Hamiltonians and their matrix elements in a perturbative manner for a wide range of quantum lattice models.
After that, we will discuss numerical techniques in chapter V based on numerical diagonalisation of finite systems that can be used to detect multi-particle bound-states and obtain series expansions for their energies.
Following that, we will discuss analytical techniques in chapter VI based on Green's function methods derived from the Dyson equation to study two-particle bound-states, that do not require exact diagonalisation. We further discuss recursion based approaches useful in the study of two-particle bound states in one-dimensional systems even when long-range interactions are present.
We will conclude with an outlook on further and future applications in chapter VII.

II Motivation

We begin with a discussion about the general structure of multi-particle spectra. Let us assume we have a particle number conserving Hamiltonian defined on a lattice. Its zero-particle spectrum, which for simplicity shall be described by a single ground state $|0\rangle$, is given by the ground-state energy $\epsilon^{(0)}$.
In general, the calculation of the exact ground state for any lattice model is highly non-trivial. We will therefore always assume that we can write our model of interest in some low energy description with regard to the energy of its lowest excitations. The calculation of these effective low energy Hamiltonians can be done using perturbative continuous unitary transformations (pCUT), which will be further elaborated on in chapter III.1. There we will discuss a perturbative approach to obtain such a low energy effective model of a quantum lattice model. This technique will also guarantee that the effective Hamiltonian is particle number conserving, as otherwise no discussion about specific particle sectors is possible.
The next sector is described by one-particle excitations. Assuming only one kind of particle we may describe it by the creation- and annihilation operators $a_{\boldsymbol{i}}^\dagger$ and a_i, which create/ destroy a particle at site $\boldsymbol{i}$ on the lattice. Again assuming a particle number conserving Hamiltonian the only actions this Hamiltonian can perform in this sector are hopping operations, destroying a particle at one site and creating a particle at another. This generic particle number conserving Hamiltonian in this sector thus takes the form

$$H^{(1)} = \epsilon^{(0)}\mathbb{1} + \sum_{\boldsymbol{i},\boldsymbol{j}} J_{\boldsymbol{i},\boldsymbol{j}} a_{\boldsymbol{i}}^\dagger a_{\boldsymbol{j}} \ . \tag{II.1}$$

Further assuming translational invariance we may always diagonalise this Hamiltonian via a Fourier transformation of the states into the momentum basis

$$a_{\boldsymbol{k}}^\dagger = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{j}} e^{\mathrm{i}\boldsymbol{j}\boldsymbol{k}} a_{\boldsymbol{j}}^\dagger \tag{II.2}$$

where N is the number of lattice sites. This leads to a dispersion relation $\omega(\boldsymbol{k})$ describing the spectrum in the one-particle sector given by $\{\epsilon^{(0)} + \omega(\boldsymbol{k}); \boldsymbol{k} \in 1.\ \text{B.Z.}\}$, where 1. B.Z. denotes the first Brillouin zone of the lattice. The one-particle spectrum of a Hamiltonian contains a plethora of information on the system as a whole, as

it usually describes the majority of its low energy physics. A property of particular interest is the energy gap $\Delta^{(1)}$ defined as the minimal energy difference between the ground state and a one-particle excitation. This property plays an important role in the theory of quantum phase transitions as a quantum phase transition is usually characterised by the closing of this gap as a function of a parameter λ of the system

$$\Delta^{(1)}(\lambda_{\text{Crit}}) = 0 \ , \tag{II.3}$$

where λ_{Crit} denotes the parameter at which the phase transition occurs (see for example [5] for more details). A common approach in the study of quantum phase transitions consists of deriving an effective low-energy particle number conserving Hamiltonian for a given quantum lattice model and afterwards calculating its one-(quasi)-particle dispersion and with it the closing of the energy gap. As previously mentioned a common technique to do so is the pCUT method.
Going beyond one-particle physics, the two-particle sector is characterised by the possible presence of two-particle interactions. In the previous second quantisation Hamiltonian these interactions are introduced as terms quartic in the number of creation- and annihilation-operators, with two creation- and two annihilation operators, i.e.

$$H^{(2)} = H^{(1)} + \sum_{\boldsymbol{i_1},\boldsymbol{i_2},\boldsymbol{i_3},\boldsymbol{i_4}} J_{\boldsymbol{i_1},\boldsymbol{i_2},\boldsymbol{i_3},\boldsymbol{i_4}} a^\dagger_{\boldsymbol{i_1}} a^\dagger_{\boldsymbol{i_2}} a_{\boldsymbol{i_3}} a_{\boldsymbol{i_4}} \ . \tag{II.4}$$

A translational symmetry again leads to the conservation of total momentum, but unlike in the one-particle sector this conserved quantity alone no longer suffices to diagonalise the Hamiltonian in this sector. This becomes clear by noting that the total momentum yields no restriction to the relative distance (or equivalently the relative momentum) between the two particles. Thus, further diagonalisation in any fixed total momentum subspace is needed. This is equivalent to the usual ansatz to reduce a two-particle problem into a centre of mass motion (here described by the total momentum) and an effective single particle in a potential, described by the interaction. The general structure of the two-particle spectrum consists of a two-particle continuum which can be interpreted as all combinations of two one-particle excitations. These continuum states will be called quasi-free, as they are not normalisable in any fixed total momentum subspace and the average distance between the two-particles is infinite on an infinite system. With the presents of interaction terms these states are usually not given by simple tensor product states of two one-particle states, which will be further discussed in chapter VI.1. Instead, they can be interpreted as scattering states. Even though the interactions may influence the states, the continuum part of the two-particle spectrum is independent of any sufficiently short-range interaction as long as the interaction operator is compact in any total momentum subspace. This is

guaranteed by Weyl's theorem (see for example [6]) for bound self-adjoint operators on a Hilbert space. The continuum spectrum is then given by the combination of all possible one-particle energies with a given total momentum $\boldsymbol{K}$

$$\epsilon^{(2)}_{\text{Continuum}}(\boldsymbol{K}) = \{\omega(\boldsymbol{K}-\boldsymbol{k}) + \omega(\boldsymbol{k}); \boldsymbol{k} \in 1.\text{ B.Z.}\}\ . \tag{II.5}$$

Besides the two-particle continuum the entire two-particle spectrum may also feature any number of bound and anti-bound states. These are normalisable states in the total momentum subspace in which they exist, have a finite average distance between the two particles and usually lie outside the continuum part of the spectrum (for a discussion of exceptions to this last point see Appendix B). During this master's thesis we will only discuss bound states explicitly, while all methods apply analogously to anti-bound states. Bound states usually only exist on a sub-region of the full 1.B.Z., whereon they can be described by a dispersion $\epsilon^{(2)}_{\text{Bound}}(\boldsymbol{k})$.
While the structure of the continuum follows from the one-particle dispersion and is thus fully described by the one particle sector, the bound-states are a distinct feature of the two-particle sector, whose existence and energy cannot be derived from the one-particle sector alone. This thesis is dedicated to the discussion of systematic methods to derive these features of the two-particle spectrum (see chapters V and VI). Looking back at quantum phase transitions, the possibility arises that a two-particle (or in general multi-particle) bound-states closes its gap to the ground-state before the one-particle excitation. This in turn would lead to a different position and behaviour of the phase transition. A systematic understanding of the behaviour of bound-state energies is therefore essential to study these possibilities (see section VI.1.4).
To illustrate the concepts discussed so far we will look at a one dimensional model of hard-core bosons, described by an onsite chemical potential $\mu > 0$, a nearest neighbour hopping term parameterised by J and a nearest neighbour density-density interaction parameterised by λ. Its full Hamiltonian is given by

$$H = \mu \sum_i n_i + J \sum_i a^\dagger_{i+1} a_i + a^\dagger_i a_{i+1} - \lambda \sum_i n_{i+1} n_i\ . \tag{II.6}$$

This Hamiltonian is already particle number conserving. The operator $n_i = a^\dagger_i a_i$ counts if a particle is present at site i. The chemical potential can be chosen such that the state with zero quasi-particles is indeed the ground state and the nearest-neighbour density-density interaction which is significant for the formation of two-particle bound-states.
The ground-state energy and dispersion of this model are readily solved for as discussed above using Fourier transformations, yielding

$$\begin{aligned} \epsilon^{(0)} &= 0 \ , \\ \omega(k) &= \mu + 2J\cos\left(k\right) \ . \end{aligned} \tag{II.7}$$

This model is integrable and thus analytically solvable in all particle sectors using the geometric Bethe ansatz [7]. Using a special case of the general geometric Bethe ansatz discussed in appendix B, we find that a two-particle bound-state is present and given by the expression

$$\begin{aligned} |\Psi_{\text{Bound}}(K)\rangle &= \sqrt{1 - 4\frac{J^2\cos^2(K/2)}{\lambda}} \sum_{m=0}^{\infty} \left(2J\frac{\cos(K/2)}{\lambda}\right)^m |K; m+1\rangle \\ \epsilon^{(2)}_{\text{Bound}}(K) &= 2\mu - \left(\lambda + 4\frac{J^2\cos^2(K/2)}{\lambda}\right) \end{aligned} \tag{II.8}$$

with the two-particle basis vectors in the total momentum subspace K

$$\begin{aligned} |K; d\rangle &= \frac{1}{\sqrt{N}} \sum_j e^{\mathrm{i}K\left(j+\frac{d}{2}\right)} |j, j+d\rangle \ , \\ |j, j+d\rangle &= a_j^\dagger a_{i+d}^\dagger |0\rangle \ . \end{aligned} \tag{II.9}$$

Note that this bound state is only normalisable for some total momenta K, which satisfy the condition

$$1 - 4\frac{J^2\cos^2(K/2)}{\lambda} > 0 \ . \tag{II.10}$$

For small values of $\lambda > 0$ the two-particle bound-state thus only exists around $K = \pi$. This becomes also clear by observing that only at $K = \pi$ the bound-state energy $\epsilon^{(2)}_{\text{Bound}}(K = \pi)$ can be written as a power series in λ around $\lambda = 0$. The non-existence of bound-states at small interaction strengths and thus the inability to obtain series expansions for their energies is a common occurrence and will be another point of discussion during this thesis. In chapter VI.1 we will develop alternative series expressions that capture theses bound-states implicitly, even if no explicit series expansion for these bound-state energies exist.
The zero- to two-particle spectrum of this model is shown in figure II.1, where the difference between the two-particle continuum and the two-particle bound state can be observed.

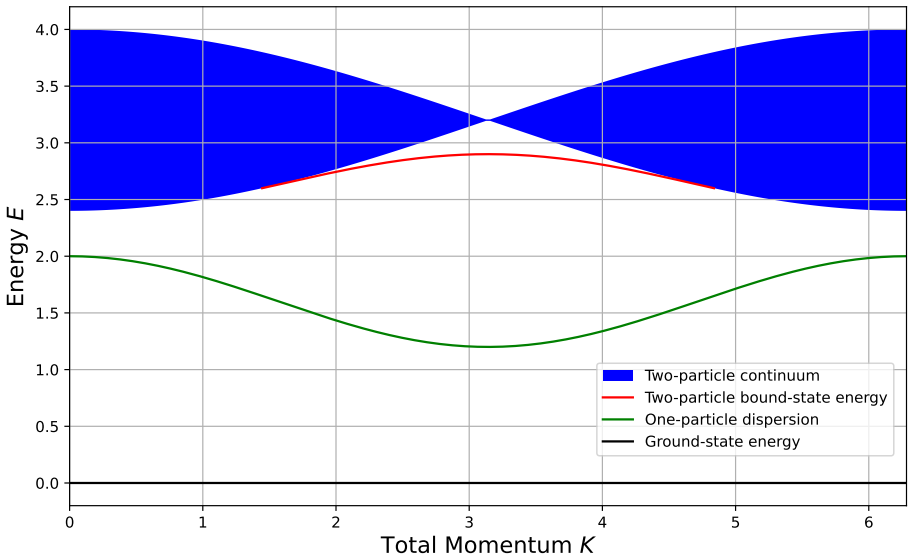

Figure II.1: Example of a spectrum of the XXZ model on a linear chain with parameters $\mu = 1.6$, $J = 0.2$ and $\lambda = 0.3$. The bound-state (red line) only exists in a subsection of the full Brillouin zone.

Continuing with the previous discussion of the multi-particle spectra in general, we notice that the three-particle and higher particle number spectra display mainly the same features as the two-particle spectra. In the sense that they contain a number of continua and potentially (anti-)bound-states of the given number of particles. The major difference between two-particle bound-states in the two-particle spectrum and n-particle bound-states in the n-particle spectrum consists of the fact that for $n > 2$ usually no reduction to an effective one-particle problem exists. While the numerical diagonalisation methods on finite systems as discussed in chapter V are applicable to any particle sector with the limit of an increase in computational demand, the analytical methods discussed in chapter VI are restricted to the two-particle sector.
As a note regarding the n-particle continuum, this does not need to be limited to a single connected continuum made of n quasi-free one-particle excitations, as now lower number bound-states can serve as one or more of the quasi-free states making up this continuum. For example if a two-particle bound-state exist (in some finite part of the B.Z.) the entire three-particle continuum can be written as a 1+1+1 continuum made out of three quasi-free one particle states and a 1+2 continuum made out of one single particle excitation and a two-particle bound-state that form a quasi-free state together. These different parts of the continuum often overlap and thus again look like a single

continuum but can still lead to significant deformations of the lower and upper edge of the continuum if compared to the always present part of the continuum made out of only single particle excitations.

III Prerequisite techniques

III.1 perturbative Continuous Unitary Transformations

The goal of this section is to give a brief introduction how a Hamiltonian can be transformed into an effective Hamiltonian with a conserved number of (quasi-)particles using continuous unitary transformations (CUT) and then be perturbatively expanded in orders of a perturbation parameter x (pCUT).
As a setup we assume a Hamiltonian of the form

$$H = H_0 + xV \tag{III.1}$$

where x is the perturbation parameter to the perturbation V and H_0 is a Hamiltonian with known eigenenergies and -states with an equidistant spectrum, captured by the counting operator Q, i.e. $[H_0, Q] = 0$. Up to constant energy shifts we may write

$$H_0 = \epsilon_0 Q \tag{III.2}$$

describing the equidistant energy spectrum with spacing ϵ_0.
This is the starting point of the perturbative expansion and it defines the notion of conserved particles as the continuous unitary transformation will transform the particles defined by Q into the adiabatically connected excitations of the full Hamiltonian H.
We further assume that we can write the perturbation in the form

$$V = \sum_{n=-N}^{N} T_n \tag{III.3}$$

where T_n changes the number of excitations counted by Q by n, i.e. $[Q, T_n] = nT_n$.
Now we want to find a unitary transformation of the whole Hamiltonian H such that the transformed Hamiltonian H_{eff} conserves the number of excitations Q

$$[H_{\text{eff}}, Q] = 0 \ . \tag{III.4}$$

Following Knetter and Uhrig [8] we introduce the notation

$$\begin{aligned} \underline{m} &= (m_1, m_2, m_3, ..., m_k) \\ m_i &\in \{0, \pm 1, \pm 2, ..., \pm N\} \\ |\underline{m}| &= k \\ T(\underline{m}) &= T_{m_1} T_{m_2} T_{m_3} ... T_{m_k} \\ M(\underline{m}) &= \sum_{i=1}^{k} m_i \end{aligned} \tag{III.5}$$

to define the infinitesimal generator of the unitary transformation

$$\eta(x;l) = \sum_{k=1}^{\infty} x^k \sum_{|\underline{m}|=k} \mathrm{sgn}(M(\underline{m})) F(l;\underline{m}) T(\underline{m}) \tag{III.6}$$

and the ansatz for the transformed Hamiltonian

$$H(x;l) = H_0 + \sum_{k=1}^{\infty} x^k \sum_{|\underline{m}|=k} F(l;\underline{m}) T(\underline{m}) \tag{III.7}$$

with a set of real functions $F(l;\underline{m})$. The functions $F(l;\underline{m})$ are determined by a set of non-linear recursive differential equations obtained by an infinitesimal step in the unitary transformation demanding

$$\partial_l H(x;l) = [\eta(x;l), H(x,l)] \ . \tag{III.8}$$

The transformation yields the desired quasi-particle conserving effective Hamiltonian when we let the parameter $l \in [0, \infty)$ go to infinity $l \to \infty$. Doing this yields the general form of the effective Hamiltonian

$$H_{\mathrm{eff}}(x) = H_0 + \sum_{k=1}^{\infty} x^k \sum_{\substack{|\underline{m}|=k \\ M(\underline{m})=0}} C(\underline{m}) T(\underline{m}) \ , \tag{III.9}$$

where $C(\underline{m}) = \lim_{l\to\infty} F(l;\underline{m})$. A list of the exact coefficients $C(\underline{m})$ can be found in [9]. Note that this technique relies on the energetic separation of the different particle number sectors and usually breaks down if different particle number sectors become degenerate, exceptions can occur if the different particle-number sectors are also separated by different conserved quantities like total spin or momentum.

III.2 Link-cluster expansion

In this section we provide an overview for the technique of linked-cluster expansions. This method is not only important for the effective calculation of results obtained via pCUT as introduced in the previous section (for details see [10]), but will also become useful for later applications in chapters V and VI.1 as it allows us to systematically and perturbatively calculate the contribution of a particle number conserving Hamiltonian acting only on a certain number of particles by splitting general matrix elements into these constituents.

III.2.1 General theory

We will summaries the works of Gelfand and Singh [11] also shown in [12] establishing a link-cluster expansion for cluster additive quantities. We start from a Hamiltonian of the form

$$H = H_0 + \lambda V \tag{III.10}$$

where H_0 defines local eigenstates that can be used as a basis and has a non-degenerate ground state $|0\rangle$. V is some term acting on more than one site with a perturbation parameter λ. In the case that the number of excitations defined by H_0 is conserved by V we may think of V as a hopping term, moving excitations between sites of the lattice. Using pCUT we may bring most Hamiltonians into this form and assume this going forward.

III.2.1.1 Cluster additivity

Following Knetter, Schmidt and Uhrig [10], given a lattice L consisting of sites and bonds between the sites (these bonds may be defined by V) we define a cluster C as a finite subset of sites and the bonds connecting the sites in the subset. A cluster is said to be linked, if there exists a path from any site included in C to any other site in C following the bonds in C. We call clusters A and B disconnected if $\mathrm{A} \cap \mathrm{B} = 0$ and $\mathrm{A} \cap \mathrm{B}$ is not linked.
Considering a cluster C and its corresponding Hilbert space $\mathbb{H}^{\mathrm{C}}$ and a quantity R^{C} defined on this cluster, we can extend this observable to the full Hilbert space $\mathbb{H}^{\mathrm{C}} \otimes \mathbb{H}^{\overline{\mathrm{C}}}$ via

$$R(\mathrm{C}) = R^{\mathrm{C}} \otimes \mathbb{1}^{\overline{\mathrm{C}}} \tag{III.11}$$

where $\overline{\mathrm{C}}$ denotes the sites not included in C.
A quantity is said to be cluster additive if for any two disconnected clusters A and B

$$R^{\mathrm{C}} = R^{\mathrm{A}} \otimes \mathbb{1}^{\mathrm{B}} + \mathbb{1}^{\mathrm{A}} \otimes R^{\mathrm{B}} \tag{III.12}$$

follows, with $\mathrm{C} = \mathrm{A} \cup \mathrm{B}$.

III.2.2 Cluster expansion

Assume we have a cluster additive quantity R. We initially assumed that the coupling between all bonds is equal to λ. We now introduce a separate coupling parameter λ_{ij} for all bonds between connected sites i and j. Next, we assume that a multi-variable expansion of R on the full lattice L in terms of these coupling parameters exist, i.e.

$$R(\mathrm{L}) = r_0 + \sum_{i,j} r_{ij}\lambda_{ij} + \sum_{ij;kl} r_{ij;kl}\lambda_{ij}\lambda_{kl} + ... \tag{III.13}$$

with the series coefficients $r_0, r_{i,j}, r_{ij;kl}, ...$ If we further assume that this series can be reordered, then we can sort terms in such a way, that we collect all terms that only contain one specific coupling parameter λ_{ij}, two specific coupling parameters $\lambda_{ij}, \lambda_{kl}$ and so on

$$R(\mathrm{L}) = r_0 + \sum_{ij}\sum_{n=1}^{\infty} a_{ij}(n)\lambda_{ij}^n + {\sum_{ij;kl}}' \sum_{n,m=1}^{\infty} a_{ij}(n,m)\lambda_{ij}^n\lambda_{kl}^m + ... \ , \tag{III.14}$$

where the primed sum denotes that λ_{ij} and λ_{kl} are distinct. We can now identify each set of bonds $ij; kl; ...$ with a cluster $\mathrm{C}_{ij;kl;...}$ containing exactly these bonds and the sites they connect. We define the weight of any given cluster $\mathrm{C}_{ij;kl;...}$ by

$$W(\mathrm{C}_{ij;kl;...}) = \sum_{n,m,...=1}^{\infty} a_{ij;kl;...}(n,m,...)\lambda_{ij}^n\lambda_{kl}^m... \tag{III.15}$$

and express $R(\mathrm{L})$ in terms of these cluster weights

$$R(\mathrm{L}) = r_0 + \sum_{N=1}^{\infty}\sum_{\mathrm{C}\in C_N} W(C) \ , \tag{III.16}$$

where C_N denotes the set of clusters containing exactly N bonds. Setting all $\lambda_{ij} = \lambda$ thus yields a cluster expansion of a quantity $R(\mathrm{L})$ defined on the full lattice, if a multi-variable expansion according to equation (III.13) exists and if the reordering according to equation (III.14) yields the same result as the original sum.

III.2.2.1 Properties of cluster weights

We want to study the properties of the cluster weights $W(\mathrm{C})$ further. Using our results so far, we find

1. The cluster weight $W(\mathrm{C})$ of a cluster C containing m bonds is of order m and higher
$$W(\mathrm{C}) = O(\lambda^m) \ . \tag{III.17}$$

2. Restricting the quantity R to any cluster C yields
$$\begin{aligned} R^{\mathrm{C}} &= r_0^{\mathrm{C}} + W(\mathrm{C}) + \sum_{c \subset \mathrm{C}} W(c) \\ W(\mathrm{C}) &= R^{\mathrm{C}} - r_0^{\mathrm{C}} - \sum_{c \subset \mathrm{C}} W(c) \end{aligned} \tag{III.18}$$
a recursive definition of the cluster weight $W(\mathrm{C})$ in terms of the quantity R^{C} evaluated on the finite cluster C and the cluster weights of the subclusters $c \subset \mathrm{C}$.

3. For a cluster C without subclusters we directly find
$$W(\mathrm{C}) = R^{\mathrm{C}} - r_0^{\mathrm{C}} \ . \tag{III.19}$$

4. Given two disconnected clusters A,B and the quantity R being cluster additive we find
$$\begin{aligned} W(\mathrm{A} \cup \mathrm{B}) &= R^{\mathrm{A}\cup\mathrm{B}} - r_0^{\mathrm{A}\cup\mathrm{B}} - \sum_{c \subset \mathrm{A}\cup\mathrm{B}} W(c) = \\ &= R^{\mathrm{A}} + R^{\mathrm{B}} - r_0^{\mathrm{A}\cup\mathrm{B}} - \sum_{c \subset \mathrm{A}\cup\mathrm{B}} W(c) = \\ &= R^{\mathrm{A}} + R^{\mathrm{B}} - r_0^{\mathrm{A}\cup\mathrm{B}} - \sum_{c \subset \mathrm{A}} W(c) - \sum_{c \subset \mathrm{B}} W(c) = \\ &= r_0^{\mathrm{A}} + \sum_{c \subset \mathrm{A}} W(c) + r_0^{\mathrm{B}} + \sum_{c \subset \mathrm{B}} W(c) - r_0^{\mathrm{A}\cup\mathrm{B}} - \sum_{c \subset \mathrm{A}} W(c) - \sum_{c \subset \mathrm{B}} W(c) = \\ &= r_0^{\mathrm{A}} + r_0^{\mathrm{B}} - r_0^{\mathrm{A}\cup\mathrm{B}} = 0 \end{aligned} \tag{III.20}$$
where we used the cluster additivity of R and the recursion equation (III.18). The last term vanishes again due to the cluster additivity of R. The cluster weight of cluster additive quantities is thus only non-zero on linked clusters.

III.2.3 Linked-cluster expansion

Combining the cluster expansion (III.16) with the result (III.20) for cluster additive quantities R we find the linked-cluster expansion

$$
\begin{aligned}
R(\mathrm{L}) &= r_0 + \sum_{M=1}^{\infty} \sum_{\substack{c \in C_M \\ C_M \text{linked}}} W(c) \\
\frac{R(\mathrm{L})}{N} &= \frac{r_0}{N} + \sum_{M=1}^{\infty} \sum_{\substack{c \in C_M \\ C_M \text{linked} \\ C_M \text{distinct}}} \mathcal{L}(c, \mathrm{L}) W(c)
\end{aligned}
\tag{III.21}
$$

where we sum over all linked clusters containing exactly M bonds that are topologically distinct. $\mathcal{L}(c, \mathrm{L})$ is called the embedding constant of the cluster c on the lattice L, which counts the number of times per site a given cluster c can be embedded on the lattice. $\frac{R(\mathrm{L})}{N}$ is the quantity R divided by the number of lattice sites N.

III.2.4 Irreducible multi-particle matrix elements

The goal of this section is the definition of cluster additive quantities related to multi-particle matrix elements. We again start from a Hamiltonian

$$H = H_0 + \lambda V \tag{III.22}$$

where we assume that H is block diagonal with respect to the number of (quasi-) particles counted by some counting operator Q. Any subspace containing a fixed number of (quasi-)particles is spanned by the states $|i_1, i_2, i_3, ...\rangle$ with (quasi-)particles at the sites i_1, i_2, i_3.... We define a corresponding matrix element as

$$h^m_{i_1,i_2,i_3,...;j_1,j_2,j_3,...} = \langle i_1, i_2, i_3, ...| \, H \, |j_1, j_2, j_3, ...\rangle \tag{III.23}$$

where m denotes the number of (quasi-)particles in the subspace. We can restrict these matrix elements to any finite cluster C via

$$h^m_{i_1,i_2,i_3,...;j_1,j_2,j_3,...}(\mathrm{C}) = \langle i_1, i_2, i_3, ...|_{\mathrm{C}} \, H^{\mathrm{C}} \, |j_1, j_2, j_3, ...\rangle_{\mathrm{C}} \tag{III.24}$$

where H^{C} only contains the sites and their connecting bonds in the cluster C. Note that the states are vectors in the Hilbert space of the cluster C.

III.2.4.1 Ground-state energy

The simplest example of these matrix elements is the ground-state energy in the sector with zero (quasi-)particles

$$h^0 = \langle 0| H |0\rangle \ . \tag{III.25}$$

Looking at two disconnected clusters A, B following the cluster additivity equation (III.12) we find

$$\begin{aligned} h^0(\mathrm{A}\cup\mathrm{B}) &= \langle 0|_{\mathrm{A}\cup\mathrm{B}} H^{\mathrm{A}\cup\mathrm{B}} |0\rangle_{\mathrm{A}\cup\mathrm{B}} = \\ &= \langle 0|_{\mathrm{A}} H^{\mathrm{A}} |0\rangle_{\mathrm{A}} \langle 0|_{\mathrm{B}} \mathbb{1}^{\mathrm{B}} |0\rangle_{\mathrm{B}} + \langle 0|_{\mathrm{A}} \mathbb{1}^{\mathrm{A}} |0\rangle_{\mathrm{A}} \langle 0|_{\mathrm{B}} H^{\mathrm{B}} |0\rangle_{\mathrm{B}} = \\ &= h^0(\mathrm{A}) + h^0(\mathrm{B}) \end{aligned} \tag{III.26}$$

the cluster additivity of the ground-state energy, where we used that $H^{\mathrm{A}\cup\mathrm{B}} = H^{\mathrm{A}} + H^{\mathrm{B}}$ and that $|0\rangle$ is a product state of the ground-state at every site, i.e. $|0\rangle_{\mathrm{A}\cup\mathrm{B}} = |0\rangle_{\mathrm{A}} \otimes |0\rangle_{\mathrm{B}}$.

III.2.4.2 One-particle matrix elements

Next, we want to investigate the properties of the matrix elements in the one-(quasi-) particle subspace

$$h^1_{i;j} = \langle i| H |j\rangle \ . \tag{III.27}$$

Again looking at two disconnected clusters A, B we find

$$\begin{aligned} h^1_{i;j}(\mathrm{A}\cup\mathrm{B}) &= \langle i|_{\mathrm{A}\cup\mathrm{B}} H^{\mathrm{A}\cup\mathrm{B}} |j\rangle_{\mathrm{A}\cup\mathrm{B}} = \langle i|_{\mathrm{A}\cup\mathrm{B}} H^{\mathrm{A}} |j\rangle_{\mathrm{A}\cup\mathrm{B}} + \langle i|_{\mathrm{A}\cup\mathrm{B}} H^{\mathrm{B}} |j\rangle_{\mathrm{A}\cup\mathrm{B}} \\ &= \begin{cases} h^1_{i;j}(\mathrm{A}) + h^0(\mathrm{B})\delta_{i;j} & i,j \in \mathrm{A} \\ h^0(\mathrm{A})\delta_{i;j} + h^1_{i;j}(\mathrm{B}) & i,j \in \mathrm{B} \\ 0 & \text{else} \end{cases} . \end{aligned} \tag{III.28}$$

If the sites i, j both lie in the same cluster A or B, then we obtain the corresponding matrix element on this cluster but on the other cluster the states $|i\rangle, |j\rangle$ are identical to the ground state on this cluster, i.e. $|i\rangle_{\mathrm{A}\cup\mathrm{B}} = |i\rangle_{\mathrm{A}} \otimes |0\rangle_{\mathrm{B}}$ for i in cluster A. Thus we conclude that the matrix elements in the one-(quasi-)particle sectors are not cluster additive.
A generalisation of the cluster additivity of the ground-state energy to the one-(quasi-) particle sector was already developed by Gelfand [13]. Instead of the pure matrix element, we define the irreducible one-particle matrix element via

$$\Delta^1_{i,j} = h^1_{i;j} - h^0\delta_{i;j} \ . \tag{III.29}$$

This quantity has the property

$$\Delta^1_{i,j}(A) = 0 \text{ for } i,j \notin A \; . \tag{III.30}$$

Using this property we can repeat the previous calculation to find

$$\begin{aligned}\Delta^1_{i,j}(\mathrm{A}\cup\mathrm{B}) &= \langle i|_{\mathrm{A}\cup\mathrm{B}}\, H^{\mathrm{A}}\, |j\rangle_{\mathrm{A}\cup\mathrm{B}} + \langle i|_{\mathrm{A}\cup\mathrm{B}}\, H^{\mathrm{B}}\, |j\rangle_{\mathrm{A}\cup\mathrm{B}} - \delta_{i;j}\left(h^0(\mathrm{A})+h^0(\mathrm{B})\right) \\ &= \begin{cases} \Delta^1_{i,j}(\mathrm{A}) & i,j\in\mathrm{A} \\ \Delta^1_{i,j}(\mathrm{B}) & i,j\in\mathrm{B} \\ 0 & \text{else} \end{cases} \\ &= \Delta^1_{i,j}(\mathrm{A}) + \Delta^1_{i,j}(\mathrm{B})\end{aligned} \tag{III.31}$$

the cluster additivity of the irreducible one-particle matrix element. Here we added zeros (III.30) to the three cases corresponding to the missing irreducible matrix elements in order to bring them into the cluster additive form.

III.2.4.3 General case: m-particle matrix elements

Analogous calculations to the one-particle matrix elements show, that the general m-particle matrix element

$$h^m_{i_1,i_2,i_3,\ldots;j_1,j_2,j_3,\ldots} = \langle i_1,i_2,i_3,\ldots|\, H\, |j_1,j_2,j_3,\ldots\rangle \tag{III.32}$$

is not cluster additive for $m>0$. A generalisation of the irreducible one-particle matrix elements can be given by

$$\Delta^m_{i_1,i_2,i_3,\ldots;j_1,j_2,j_3,\ldots} = h^m_{i_1,i_2,i_3,\ldots;j_1,j_2,j_3,\ldots} - \sum_{n=1}^{m} A^n_{i_1,i_2,i_3,\ldots;j_1,j_2,j_3,\ldots} \tag{III.33}$$

with the quantities

$$\begin{aligned}A^n_{i_1,\ldots,i_m;j_1,\ldots,j_m} = \sum_{k_1<k_2<\ldots<k_n}^{m}\; \sum_{l_1<l_2<\ldots<l_n}^{m} & \Delta^{m-n}_{i_1,\ldots,\widehat{i_{k_1}},\ldots,\widehat{i_{k_n}},\ldots,i_m;j_1,\ldots,\widehat{j_{l_1}},\ldots,\widehat{j_{k_n}},\ldots,j_m} \\ & \times\delta_{i_{k_1},\ldots,i_{k_n};j_{l_1},\ldots,j_{l_n}}\end{aligned} \tag{III.34}$$

where the hat $\widehat{i_{k_1}}$ denotes that this index is no longer present in the state and $\Delta^0 = h^0$. Note that the Kronecker-delta $\delta_{i_{k_1},\ldots,i_{k_n};j_{l_1},\ldots,j_{l_n}}$ checks only if the sets $i_{k_1},\ldots,i_{k_n}$ and

$j_{l_1}, ..., j_{l_n}$ are equal as sets regardless of their ordering.
We can invert this formula to obtain an expression for the irreducible matrix elements containing only regular matrix elements similarly to expression (III.33) but with alternating signs

$$\Delta^m_{i_1,i_2,i_3,...;j_1,j_2,j_3,...} = h^m_{i_1,i_2,i_3,...;j_1,j_2,j_3,...} + \sum_{n=1}^{m} (-1)^n \tilde{A}^n_{i_1,i_2,i_3,...;j_1,j_2,j_3,...}, \tag{III.35}$$

where $\tilde{A}^n_{i_1,i_2,i_3,...;j_1,j_2,j_3,...} = A^n_{i_1,i_2,i_3,...;j_1,j_2,j_3,...}(\Delta \leftrightarrow h)$ just replaced the irreducible matrix elements with the regular matrix elements. A prove of the cluster additivity can be found in appendix A.

III.2.4.4 Properties of the irreducible m-particle matrix elements

We find the following properties for the irreducible m-particle matrix elements:

1. $\Delta^m_{i_1,i_2,i_3,...;j_1,j_2,j_3,...}$ is cluster additive.
2. $\Delta^m_{i_1,i_2,i_3,...;j_1,j_2,j_3,...}(\mathrm{A}) = 0$ if $\{i_1, i_2, i_3, ...; j_1, j_2, j_3, ...\} \not\subset \mathrm{A}$.
3. $\Delta^m_{i_1,i_2,i_3,...;j_1,j_2,j_3,...}(\mathrm{A} \cup \mathrm{B}) = \Delta^m_{i_1,i_2,i_3,...;j_1,j_2,j_3,...}(\mathrm{A})$ if $\{i_1, i_2, i_3, ...; j_1, j_2, j_3, ...\} \subset \mathrm{A}$ and vice versa for B.
4. $\Delta^m_{i_1,i_2,i_3,...;j_1,j_2,j_3,...}$ is the contribution to the matrix element $h^m_{i_1,i_2,i_3,...;j_1,j_2,j_3,...}$ that originates from terms in V that move exactly m particles at once, i.e. that contain exactly m creation- and annihilation operators.

Property 4 will be especially important in chapters V and VI.1 where we use this to separate the Hamiltonian into a free Hamiltonian containing only hopping terms determined by $\Delta^1_{i;j}$ and two-particle interaction terms described by $\Delta^2_{i_1,i_2;j_1,j_2}$.

IV Example Models

In this chapter we will introduce two models that will be used throughout this master thesis as examples and tests for several of the methods discussed in the later chapters V and VI.

IV.1 XXZ-Model

The XXZ-Model on a lattice L is defined as a model of spin-1/2 particles described by the Hamiltonian

$$H = \sum_{<i,j>\in L} J\left(S_i^x S_j^x + S_i^y S_j^y\right) + \lambda S_i^z S_j^z \ , \tag{IV.1}$$

where $S^{x/y/z}$ denote the spin-1/2 operators. Using the mapping

$$\begin{aligned} S_i^x &= \frac{1}{2}\left(a_i^\dagger + a_i\right) \\ S_i^y &= \frac{1}{2\mathrm{i}}\left(a_i^\dagger - a_i\right) \end{aligned} \tag{IV.2}$$

to hard-core bosons, we may rewrite the model up to a constant energy shift as

$$H_{\mathrm{XXZ}} = \frac{J}{2} \sum_{<i,j>\in L} a_i^\dagger a_j + a_j^\dagger a_i - \lambda \sum_{<i,j>\in L} n_i n_j \tag{IV.3}$$

with $n_i = a_i^\dagger a_i$, the hopping amplitude J, and the interaction strength λ. Sums over all sites and their nearest neighbours are denoted by $\sum_{<i,j>\in L}$. Notable limits of this model include the Heisenberg model in the limit $J = \lambda$, the Ising model in the limit $J = 0$ and the XY-model for $\lambda = 0$. In the following sections we will discuss some variants of this model and their bound-state properties.

IV.1.1 1d XXZ-Model

The XXZ-Model defined on a linear chain was already mentioned in chapter II. It is of special interest as it is integrable and exactly solvable using the Bethe ansatz [7]. In hard-core boson language its Hamiltonian reads

$$H = \frac{J}{2} \sum_i a_{i+1}^\dagger a_i + a_i^\dagger a_{i+1} - \lambda \sum_i n_{i+1} n_i \ . \tag{IV.4}$$

As we are interested in its bound-states we introduce the n-particle basis

$$|i_1, ..., i_n\rangle = a_{i_1}^\dagger ... a_{i_n}^\dagger \, |0\rangle \tag{IV.5}$$

where $|0\rangle$ is the state without hard-core bosons. Next one introduces the n-particle basis

$$|K; d_1, ..., d_{n-1}\rangle = \frac{1}{\sqrt{N}} \sum_j e^{\mathrm{i}K\left(j + \frac{1}{n}\sum_{l=1}^{n-1}(n-l)d_l\right)} \left| j, j+d_1, ..., j + \sum_{l=1}^{n-1} d_l \right\rangle \tag{IV.6}$$

with the system size N, the total momentum K of all particles and the positive distances between the particles $d_1, ..., d_{n-1} > 0$. Here the distance d_j is the distance between the j-th and $j+1$-th particle. Using this basis it is sufficient to make the ansatz

$$|\Psi_{\text{Bound}}(K)\rangle \propto \sum_{d_1,...,d_{n-1}=1}^{\infty} A_1^{d_1} ... A_{n-1}^{d_{n-1}} \, |K; d_1, ..., d_{n-1}\rangle \tag{IV.7}$$

with complex numbers $A_1, ..., A_{n-1}$ to obtain the n-particle bound-states of this model. This ansatz is a special case of the general geometric Bethe ansatz and only yields the bound-states of the model. A full discussion of this ansatz and its solutions is given in Appendix B. For this master thesis we will focus our attention onto the two- and three-particle bound-states of this model, obtained via the above ansatz. As mentioned in chapter II the two-particle bound-state is given by

$$\begin{aligned}
\left|\Psi^{(2)}_{\text{Bound}}(K)\right\rangle &= \sqrt{1-\frac{J^2\cos^2(K/2)}{\lambda^2}}\sum_{m=0}^{\infty}\left(J\frac{\cos(K/2)}{\lambda}\right)^m|K;m+1\rangle \\
\epsilon^{(2)}_{\text{Bound}}(K) &= -\left(\lambda+\frac{J^2\cos^2(K/2)}{\lambda}\right) \\
0 &< 1-\frac{J^2\cos^2(K/2)}{\lambda^2}
\end{aligned} \tag{IV.8}$$

with the corresponding eigenstate, eigenenergy, and the normalisation condition for which the eigenstate is normalisable in the total momentum K subspace.
Likewise, for three particles one obtains

$$\begin{aligned}
\left|\Psi^{(3)}_{\text{Bound}}(K)\right\rangle &\propto \sum_{d_1,d_2=1}^{\infty} A^{d_1}\overline{A}^{d_2}\,|K;d_1,d_2\rangle \\
A &= e^{-\mathrm{i}K/3}\frac{\lambda/J-e^{\mathrm{i}K}}{1-(\lambda/J)^2} \\
\epsilon^{(3)}_{\text{Bound}}(K) &= -\left(2\lambda+2\frac{J\cos(K)-\lambda}{1-(\lambda/J)^2}\right) \\
0 &< 1-\frac{(\lambda/J)^2-2\cos(K)\lambda/J+1}{\left(1-(\lambda/J)^2\right)^2}\,,
\end{aligned} \tag{IV.9}$$

where $\overline{A}$ denotes the complex conjugate of A. These analytical results will be used in chapter V to compare them with numerical techniques and in chapter VI.1 to test whether they can be reproduced by the Green's function technique.

IV.1.2 2d XXZ-Model

Defined on a two-dimensional square lattice the XXZ-Model (IV.3) is no longer exactly solvable, though it is still one of the simplest examples for a two-dimensional system with two-particle bound-states. After again introducing the two dimensional analogy of the (K,d)-basis

$$|\boldsymbol{K};\boldsymbol{d}\rangle = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{j}} e^{\mathrm{i}K(\boldsymbol{j}+\boldsymbol{d}/2)}\,|\boldsymbol{j},\boldsymbol{j}+\boldsymbol{d}\rangle \tag{IV.10}$$

we find that the hopping term vanishes identically at the point $\boldsymbol{K}=(\pi,\pi)$ in the Brillouin-zone. Thus we obtain two trivial two-particle bound-states

$$\begin{aligned}\left|\Psi^{(2)}_{\text{Bound,x}}(\boldsymbol{K}=(\pi,\pi))\right\rangle &= |\boldsymbol{K}=(\pi,\pi);\boldsymbol{d}=(1,0)\rangle \\ \left|\Psi^{(2)}_{\text{Bound,y}}(\boldsymbol{K}=(\pi,\pi))\right\rangle &= |\boldsymbol{K}=(\pi,\pi);\boldsymbol{d}=(0,1)\rangle \\ \epsilon^{(2)}_{\text{Bound,x/y}}(\boldsymbol{K}=(\pi,\pi)) &= -\lambda\end{aligned} \tag{IV.11}$$

with degenerate energies. As in the one-dimensional case it is expected that this is the only point in the Brillouin-zone where a two-particle bound-state exists for arbitrarily small values of the NN-density-density interaction λ. In chapter VI.1.7 we will derive an exact implicit equation for all two-particle bound-state energies of this model at arbitrary values of the total momentum $\boldsymbol{K}$, where this will serve as a two-dimensional example.

IV.1.3 1d Long-range XXZ-Model

We also introduce a generalised long-range version of the one dimensional XXZ-model

$$H = -\frac{J}{2}\sum_i a^\dagger_{i+1}a_i + a^\dagger_i a_{i+1} - \sum_i\sum_{r=1}^{\infty}\lambda(r)n_{i+r}n_i \tag{IV.12}$$

where the long-range nature is only present in the density-density interaction, while the hopping terms stays nearest neighbour. In chapter VI.2 we will discuss a general procedure how the two-particle bound-states in this model can be studied. A notable version of this model includes the case $\lambda(r) = V/r$ with some constant V, in which case the model corresponds to a one-dimensional discrete version of the hydrogen atom whose bound-states are already known [14].

IV.2 Heisenberg Ladder

The antiferromagnetic Heisenberg model on a ladder geometry is defined via the Hamiltonian

$$H = J_\parallel\left(\sum_{i=1}^{N}\boldsymbol{S}_{i,A}\boldsymbol{S}_{i+1,A} + \sum_{i=1}^{N}\boldsymbol{S}_{i,B}\boldsymbol{S}_{i+1,B}\right) + J_\perp\sum_{i=1}^{N}\boldsymbol{S}_{i,A}\boldsymbol{S}_{i,B} \tag{IV.13}$$

with positive couplings $J_\parallel, J_\perp > 0$ along the two legs A, B and the rungs of the ladder.

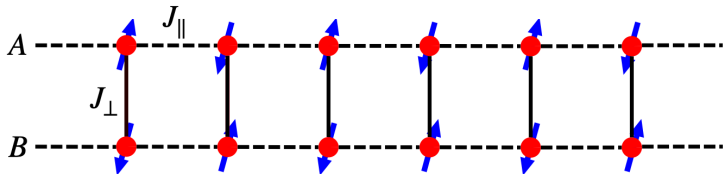

Figure IV.1: Heisenberg ladder with couplings $J_\parallel$ along the legs A, B and $J_\perp$ perpendicular to them.

Spin ladder systems like these have long been studied in the context of gapped spin systems and superconductivity in the case of additional doping [15][4]. In contrast to the Heisenberg chain no exact solutions are known, though exactly solvable modifications of this model exist, which can reproduce some limiting behaviours [16].
We will study this model using a dimer expansion out of the strong coupling limit $J_\parallel/J_\perp = x \ll 1$. In the limit $x = 0$ the coupling along the ladder's legs vanishes and the system is given by decoupled rung dimers. Due to the antiferromagnetic coupling between the two spins in each dimer they are described by a singlet ground state and three degenerate local excited states, which will be called triplets

$$\begin{aligned} H_{\text{dimer}} &= J_{\text{rung}} \boldsymbol{S}_A \boldsymbol{S}_B \\ H_{\text{dimer}} \frac{1}{\sqrt{2}} \left(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle\right) &= -\frac{3}{4} J_{\text{rung}} \frac{1}{\sqrt{2}} \left(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle\right) \\ H_{\text{dimer}} |\uparrow,\uparrow\rangle &= \frac{1}{4} J_{\text{rung}} |\uparrow,\uparrow\rangle \\ H_{\text{dimer}} |\downarrow,\downarrow\rangle &= \frac{1}{4} J_{\text{rung}} |\downarrow,\downarrow\rangle \\ H_{\text{dimer}} \frac{1}{\sqrt{2}} \left(|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle\right) &= \frac{1}{4} J_{\text{rung}} \frac{1}{\sqrt{2}} \left(|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle\right) \ . \end{aligned} \tag{IV.14}$$

If leave the rung dimer limit $x = 0$, these triplets will no longer be the exact excitations of the system. Instead for sufficiently small values of x the true excitations will be dressed versions of these triplets, which we will call triplons. Regarding bound-states the antiferromagnetic Heisenberg ladder is known to posses two-triplon bound-states [2] and is suspected to possess three-triplon bound-states in the strong coupling limit [3].

IV.2.1 Triplet picture

Based on the eigenstates of the isolated dimers and the total spin operator $\boldsymbol{S}_{\text{tot}} = \boldsymbol{S}_A + \boldsymbol{S}_B$ we can label the dimer states by their total spin eigenvalue $\boldsymbol{S}^2_{\text{tot}}$ and total spin z-component $(\boldsymbol{S}_{\text{tot}})_{\text{z}}$

$$\begin{aligned} |1,1\rangle &\equiv |\uparrow,\uparrow\rangle \\ |1,0\rangle &\equiv \frac{1}{\sqrt{2}}\left(|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle\right) \\ |1,-1\rangle &\equiv |\downarrow,\downarrow\rangle \\ |0,0\rangle &\equiv \frac{1}{\sqrt{2}}\left(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle\right) \ , \end{aligned} \tag{IV.15}$$

where $|0,0\rangle$ is the antiferromagnetic dimer ground state. We can readily define triplet creation operators which create the three kinds of excitations from the ground state

$$\begin{aligned} t^{1,\dagger}\,|0,0\rangle &= |1,1\rangle \\ t^{0,\dagger}\,|0,0\rangle &= |1,0\rangle \\ t^{-1,\dagger}\,|0,0\rangle &= |1,-1\rangle \end{aligned} \tag{IV.16}$$

which can be expressed using the spin operators as follows

$$\begin{aligned} t^{1,\dagger} = |1,1\rangle\langle 0| &= \frac{1}{\sqrt{2}} S_A^+ S_B^+ \left(S_A^- - S_B^-\right) \\ t^{0,\dagger} = |1,0\rangle\langle 0| &= \frac{1}{2}\left(S_A^+ + S_B^+\right)\left(S_A^- - S_B^-\right) \\ t^{-1,\dagger} = |1,-1\rangle\langle 0| &= \frac{1}{\sqrt{2}}\left(S_A^- - S_B^- + (S_A^+ - S_B^+) S_A^- S_B^-\right) \ , \end{aligned} \tag{IV.17}$$

where we introduced the spin-$\frac{1}{2}$ creation and annihilation operators $S^{\pm} = S^x \pm i S^y$. The inverse transformation is given by

$$\begin{aligned} S_A^+ &= \frac{1}{\sqrt{2}}\left(-t^{1,\dagger} + t^{-1} + t^{1,\dagger}t^0 + t^{0,\dagger}t^{-1}\right) \\ S_B^+ &= \frac{1}{\sqrt{2}}\left(t^{1,\dagger} - t^{-1} + t^{1,\dagger}t^0 + t^{0,\dagger}t^{-1}\right) \ . \end{aligned} \tag{IV.18}$$

These triplet operators form a hard-core boson algebra.
The full Hamiltonian can be rewritten in terms of triplet operators as

$$
\begin{aligned}
&\boldsymbol{S}_{i,A}\boldsymbol{S}_{i,B} = -\frac{3}{4} + \sum_{\gamma\in\{1,0,-1\}} n_i^\gamma \\
&\boldsymbol{S}_{i,A}\boldsymbol{S}_{i+1,A} + \boldsymbol{S}_{i,B}\boldsymbol{S}_{i+1,B} = \\
&= \frac{1}{2}\sum_{\gamma\in\{1,0,-1\}} t_i^{\gamma,\dagger}t_{i+1}^{\gamma} + t_{i+1}^{\gamma,\dagger}t_i^{\gamma} \\
&+ \frac{1}{2}\left(t_i^{1,\dagger}t_{i+1}^{0,\dagger}t_i^0t_{i+1}^1 + t_i^{1,\dagger}t_{i+1}^{-1,\dagger}t_i^0t_{i+1}^0 + t_i^{0,\dagger}t_{i+1}^{0,\dagger}t_i^{-1}t_{i+1}^1 + t_i^{0,\dagger}t_{i+1}^{-1,\dagger}t_i^{-1}t_{i+1}^0\right) + h.c. \\
&+ \frac{1}{2}\left(n_i^1n_{i+1}^1 + n_i^{-1}n_{i+1}^{-1} - n_i^1n_{i+1}^{-1} - n_i^{-1}n_{i+1}^1\right) \\
&+ \frac{1}{2}\sum_{\gamma\in\{1,0,-1\}} e^{i\pi\gamma}\left(t_i^{\gamma,\dagger}t_{i+1}^{-\gamma,\dagger} + t_{i+1}^{-\gamma}t_i^{\gamma}\right) \ .
\end{aligned}
\tag{IV.19}
$$

Here we introduced the notation $n_i^\alpha = t_i^{\alpha,\dagger}t_i^\alpha$. The term $\boldsymbol{S}_{i,A}\boldsymbol{S}_{i,B}$ corresponds to the local triplet energy. The term $\boldsymbol{S}_{i,A}\boldsymbol{S}_{i+1,A} + \boldsymbol{S}_{i,B}\boldsymbol{S}_{i+1,B}$ describes the hopping of single triplets and interaction of two neighbouring triplets as well as non-triplet number conserving terms.
Using pCUT we can perturbatively derive a particle number conserving Hamiltonian describing the low energy physics of this model. In the pCUT language we may write the Heisenberg ladder Hamiltonian as

$$
\begin{aligned}
H/J_\parallel &= H_0 + xV \\
H_0 &= -\frac{3}{4}N + \sum_{i=1}^{N}\sum_{\gamma\in\{1,0,-1\}} t_i^{\gamma,\dagger}t_i^{\gamma} \\
V &= \sum_{i=1}^{N} T_{-2} + T_0 + T_2 \\
T_0 &= \frac{1}{2}\sum_{\gamma\in\{1,0,-1\}} t_i^{\gamma,\dagger}t_{i+1}^{\gamma} + t_{i+1}^{\gamma,\dagger}t_i^{\gamma} \\
&\quad + \frac{1}{2}\left(t_i^{1,\dagger}t_{i+1}^{0,\dagger}t_i^0t_{i+1}^1 + t_i^{1,\dagger}t_{i+1}^{-1,\dagger}t_i^0t_{i+1}^0 + t_i^{0,\dagger}t_{i+1}^{0,\dagger}t_i^{-1}t_{i+1}^1 + t_i^{0,\dagger}t_{i+1}^{-1,\dagger}t_i^{-1}t_{i+1}^0\right) + h.c. \\
&\quad + \frac{1}{2}\left(n_i^1n_{i+1}^1 + n_i^{-1}n_{i+1}^{-1} - n_i^1n_{i+1}^{-1} - n_i^{-1}n_{i+1}^1\right) \\
T_2 &= \frac{1}{2}\sum_{\gamma\in\{1,0,-1\}} e^{i\pi\gamma}t_i^{\gamma,\dagger}t_{i+1}^{-\gamma,\dagger} = T_{-2}^\dagger \ .
\end{aligned}
\tag{IV.20}
$$

IV.2.2 Three-particle total spin-0 subspace

In light of the three-particle bound-states of this model [3] it is useful to look at specific total spin-sectors. As each triplet excitation acts as a spin-1 particle we can combine two of those to form either a total spin 0,1, or 2 state. It is known [2] that the two-triplet total spin-0 and spin-1 subspace contains a bound-state each and the two-triplet total spin-2 subspace contains an antibound-state. For the three-triplet sector we can form either a total spin 0, 1, 2 or 3 state. The Heisenberg interactions along each bond conserve these total spin state subspaces and it is expected that due to the antiferromagnetic nature of the interaction the total spin-0 subspace contains the lowest lying three-particle states, as in the two-particle case. Using the usual Clebsch-Gordan-coefficients we find a unique way to combine three spin-1 states to a spin-0 sate via

$$|a,b,c\rangle^0 = \frac{1}{\sqrt{6}}\left(t^{1,\dagger}_{[a}t^{-1,\dagger}_{b}t^{0,\dagger}_{c]}\right)|0\rangle \ , \tag{IV.21}$$

where a, b, c denote the positions of the three triplets and $[a, b, c]$ denotes their total antisymmetrisation without additional factors. Due to the indistinguishability of the triplets we can restrict these states to $a < b < c$. In this subspace we can thus map the system to a system of three identical hard-core bosons. In first order of the perturbation $x = J_\parallel/J_\perp$ the effective Hamiltonian takes the form

$$H_{\text{eff}} = H_0 + \frac{x}{2}\left(\sum_{\alpha\in\{-1,0,1\}}\sum_{j=1}^{N} t^{\alpha,\dagger}_{j+1}t^{\alpha}_{j} + h.c. - \sum_{i=1}^{N} n_i n_{i+1}\right) + O(x^2) \tag{IV.22}$$

with $n_i = n_i^1 + n_i^0 + n_i^{-1}$. This Hamiltonian only contains NN-hopping terms and NN-density-density interactions. In the spin-0 sector we can map this onto the three particle sector of the XXZ-Model on a linear chain. The results (IV.9) for the three-particle bound-state of the XXZ-model in the special case $\lambda = J = x/2$ then yield

$$\left|\Psi^{(3)}_{\text{Bound}}\right\rangle = 3\sum_{d,d'=1}^{\infty}\left(-\frac{1}{2}\right)^{d+d'}|0;d,d'\rangle \tag{IV.23}$$

with an energy of

$$\epsilon^{(3)}_{\text{bound}} = \frac{9}{4} - \frac{3}{2}x + O(x^2) \ . \tag{IV.24}$$

In first order this state only exists at a centre of mass momentum of exactly $K = 0$ and is energetically degenerate with the lower edge of the three particle continuum.

Due to this fact one can only hope to obtain a series expansion of this states energy at a total momentum of $K = 0$ and even there a series expansion is not easily obtained as will be discussed in a later chapter V.2.1.

IV.2.3 Heisenberg ladder with additional cross terms

As a variation of the typical Heisenberg ladder we further introduce the Heisenberg ladder with cross terms

$$\begin{aligned} H = J_{\parallel} \left(\sum_{i=1}^{N} \boldsymbol{S}_{i,A} \boldsymbol{S}_{i+1,A} + \sum_{i=1}^{N} \boldsymbol{S}_{i,B} \boldsymbol{S}_{i+1,B} \right) + \\ + J_{\mathrm{X}} \left(\sum_{i=1}^{N} \boldsymbol{S}_{i,A} \boldsymbol{S}_{i+1,B} + \sum_{i=1}^{N} \boldsymbol{S}_{i,A} \boldsymbol{S}_{i+1,B} \right) + J_{\perp} \sum_{i=1}^{N} \boldsymbol{S}_{i,A} \boldsymbol{S}_{i,B} \ . \end{aligned} \tag{IV.25}$$

After division by $J_{\perp}$ we can again expand this model into an effective Hamiltonian out of the dimer limit using pCUT. This model will serve as an example for a model with two-perturbative parameter $x_1 = J_{\parallel}/J_{\perp}$ and $x_2 = J_{\mathrm{X}}/J_{\perp}$. In the later chapter VI.1.7 we will calculate the two-triplon bound-states of this model using the Green's function method from chapter VI.1.

V Numerical Diagonalisation methods for multi-particle bound-state energies

Using the previously discussed techniques of irreducible matrix elements calculated using the pCUT approach, setup as a linked-cluster expansion, we are capable to obtain the matrix elements of a wide range of effective Hamiltonians up to high orders in one or more expansion parameters. These effective Hamiltonians can be viewed as low-energy descriptions and allow us to describe this model in a particle number conserving way, where the particles that are conserved are adiabatically connected to those determined by the unperturbed limit of the pCUT expansion (III.2). Due to this particle number conservation the Hilbert-space of a given particle sector grows only polynomial in the number of lattice sites in contrast to the exponential growth for a non-particle conserving Hamiltonian and thus allows us the study of large finite systems with periodic boundary conditions. The study of large finite systems is usually not required in the one-particle sector as the translational invariance guaranties diagonalisation up to flavour mixing via a Fourier transformation, the two- and higher-number of particle sectors do not admit a general diagonalisation scheme. While the two-particle sector allows for some additional analytic techniques which operate fully in the thermodynamic limit (see chapter VI), we are often limited to the restriction of calculating matrix elements to large but finite systems.
An immediate application of the pCUT and linked-cluster expansion results consists of the numerical diagonalisation (short ND) of the effective Hamiltonian for some fixed values of the perturbation parameters on a finite system. This method allows us to study the general structure of the given particle sector and is often useful to determine whether or not a bound-state exists at all, but is limited if we are interested in the behaviour of the bound-state as a function of the perturbative parameters. This method only allows us to sample the model at a number of perturbation values and is bound to fail if the convergence of the effective Hamiltonian worsens, as it does not admit a systematic way of extrapolating the results obtained for small, convergent values of the perturbation parameter to larger values. We therefore want to discuss how we can obtain series expansions of multi-particle bound-states using results obtained from ND, allowing us to extrapolate these results up to a point of quantum phase transition using extrapolation techniques like Padé or Dlogpadé expansions [17].
In this chapter we will discuss how numerical diagonalisation in large systems can

be used to obtain these extrapolatable results for multi-particle bound-states in any system described by an effective particle number conserving Hamiltonian.

V.1 Bound-state series expansions using Rayleigh-Schrödinger perturbation theory

Besides the direct calculation of the bound-state energy from an effective Hamiltonian as discussed in the previous section, we are often interested in series expansions of these bound-state energies in orders of the perturbation parameters. In this section we will discuss the calculation of these energies using Rayleigh-Schrödinger perturbation theory on finite lattices using ND.
In the context of bound-states, starting from the limit of free particles, we face a dilemma with this ansatz. A perturbative series expansion requires a starting point to expand around. If we choose the undisturbed Hamiltonian as starting point, we are unable to obtain a series expansion for the potential bound-states, as bound-states do not exist in the limit of free particles. To combat this problem we instead look at the Hamiltonian in its first non-trivial order. Meaning that all previous orders of the Hamiltonian are proportional to the identity on the Hilbert-space we are interested in. As an example in the context of pCUT the zeroth order is given by the particle counting operator chosen for the pCUT expansion. Since we look at a sector with a fixed particle number this is a multiple of the identity and the first non-trivial order is usually given by the first order effective Hamiltonian.
Starting from an effective Hamiltonian of the form

$$H(x) = \sum_{n=0}^{M} H^{(n)} x^n \tag{V.1}$$

we remove all orders up to the first non-trivial order r

$$\begin{aligned} H(x) &= \sum_{n=0}^{M} H^{(n)} x^n = \sum_{n=0}^{r-1} h^{(n)} x^n \mathbb{1} + x^r \sum_{n=r}^{M} H^{(n)} x^{n-r} \\ H(x) &\to \sum_{n=0}^{M-r} H^{(n+r)} x^n = \sum_{n=0}^{M-r} \tilde{H}^{(n)} x^n \ , \end{aligned} \tag{V.2}$$

where $h^{(n)}$ are scalars that can be added to the finial expansion in the end. After dropping the trivial orders, we split this newly obtained Hamiltonian such that the first non-trivial order is the undisturbed Hamiltonian and the rest is a perturbation

$$H(x) = \sum_{n=0}^{M-r} \tilde{H}^{(n)} x^n = \tilde{H}^{(0)} + xV(x) \ . \tag{V.3}$$

From this point we can perform perturbation theory on a finite lattice of size N. Using ND we obtain a full finite set of eigenstates and energies of the undisturbed Hamiltonian $\tilde{H}^{(0)}$

$$\tilde{H}^{(0)} \left|\Psi_j^{(0)}\right\rangle = E_j^{(0)} \left|\Psi_j^{(0)}\right\rangle \ . \tag{V.4}$$

Afterwards, we can use the formulas of Rayleigh-Schrödinger perturbation theory to calculate a series expansion for any of the states obtained via ND

$$\begin{aligned}
\left|\Psi_m^{(n+1)}\right\rangle &= \frac{1}{E_m^{(0)} - \tilde{H}^{(0)}} P_m^{(0)} \left(V(x) \left|\Psi_m^{(n)}\right\rangle - \sum_{j=1}^{n-1} E_m^{(j)} \left|\Psi_m^{(n-j)}\right\rangle \right) \ , \\
E_m^{(n+1)} &= \left\langle \Psi_m^{(0)} \right| V(x) \left|\Psi_m^{(n)}\right\rangle \ , \\
E_m &= \sum_{n=0}^{\infty} E_m^{(n)} x^n \ , \\
|\Psi_m\rangle &= \sum_{n=0}^{\infty} x^n \left|\Psi_m^{(n)}\right\rangle \ ,
\end{aligned} \tag{V.5}$$

where we used the projection operator $P_m^{(0)} = \mathbb{1} - \left|\Psi_m^{(0)}\right\rangle \left\langle \Psi_m^{(0)} \right|$. In the case that $V(x)$ is still a series in x one has to collect all terms of a given order when calculating E_m. Note that all of the above calculations are performed on a finite lattice with N lattice sites and at a fixed value of the total momentum K. Therefore, all series expansion coefficients $E_m^{(n)}(N)$ have to be seen as functions of the system size. If we are interested in the series expansion in the thermodynamic limit $N \to \infty$ we have to solve two problems:
The first problem consists in selecting the same bound-state when we change the system size N. Almost all states obtained via ND will converge towards continuum states and therefore their energetic difference will also vanish in the limit $N \to \infty$. A naive way of obtaining a bound-state from this large set of states obtained via the ND consists of choosing the lowest energy eigenstate. This can become problematic if either multiple bound-states are present or if the bound-state's energy is only just below the continuum (for example if one wants to investigate the point in total momentum K space where the bound-state vanishes into the continuum). A more systematic way

will be discussed in section V.2 where bound-states will be identified via the scaling of their average distance expectation values.
The second problem arising, if we are able to identify corresponding bound-states from the set of all eigenstates obtained via ND for different system sizes N, is the extrapolation of the coefficients as functions of the system size N to the thermodynamic limit. Usually these coefficients converge quickly even for small system sizes otherwise a scaling ansatz and a function fit can be applied. Series coefficients often display a power law behaviour for their scaling in the system size N. We will therefore assume that the coefficients as functions of the system size N behave like

$$E_m^{(n)}(N) = E_m^{(n)}(\infty) + \alpha N^{-\beta} \tag{V.6}$$

where $E_m^{(n)}(\infty)$ is the desired value of the expectation value in the thermodynamic limit and α, β are free parameters. After calculating $E_m^{(n)}(N)$ for a range of system sizes N one can obtain the thermodynamic limit $E_m^{(n)}(\infty)$ by fitting the above function ansatz to the set of calculated values.
Regarding the radius of convergence of these perturbative series, we deal with two potential limiting factors. First is the initial radius of convergence of the effective model used as a starting point. Second is the possibility that a multi-particle bound-state vanishes at some critical value of the perturbation x_c usually because it overlaps with a multi-particle continuum. In this case the full bound-state energy can only be formally defined in the range $x = 0$ to $x = x_c$ and any perturbative approximation of it is expected to fail approaching x_c.

V.1.1 Examples

V.1.1.1 Heisenberg ladder two-triplon bound-states

We will use the Heisenberg ladder introduced in IV.2 to test this ansatz. For the two-triplon bound-state energies a similar ansatz as discussed in the previous chapter was used in reference [2] to calculate the energies up to twelfth-order. These results will be used as comparison. We will look at the total spin-0 sector where a bound-state is known to exist. Using the Clebsch-Gordan coefficients we can combine two triplons to form a total spin-0 state as

$$|a,b\rangle^0 = \frac{1}{\sqrt{3}}\left(t_a^{1,\dagger}t_b^{-1,\dagger} - t_a^{0,\dagger}t_b^{0,\dagger} + t_a^{-1,\dagger}t_b^{1,\dagger}\right)|0\rangle \ . \tag{V.7}$$

Since there is only one way two combine two spin-1 particles to a spin-0 particle we may again map this to a system of two hard-core bosons (identical to the discussion of

the three-triplet total spin-0 sector V.1.1.2). The first-order effective Hamiltonian in this subspace thus takes the form

$$H_{\text{eff}} = H_0 + \frac{x}{2}\left(\sum_{\alpha\in\{-1,0,1\}}\sum_{j=1}^{N} t_{j+1}^{\alpha,\dagger}t_j^{\alpha} + h.c. - 2\sum_{i=1}^{N} n_i n_{i+1}\right) + O(x^2)\ , \tag{V.8}$$

which again corresponds to the XXZ model with a ratio $\lambda/J = -2$. Looking at the two-particle bound-state condition of the XXZ model (IV.8) we notice that in first order this bound-state exists at every value of the total momentum K. Using this first-order as our first non-trivial order we are able to perform a series expansion at every value of the total momentum K. Tables V.1 and V.2 depict the first four expansion coefficients for different system sizes N at total momenta $K = \pi$ and $K = \frac{3}{4}\pi$ respectively. Notice that even at a system size of 20 sites (rung dimers in the original model) the coefficients are already well converged so no extrapolation is necessary.

N	10	20	30	40	50
$c_1(K=\pi)$	-1	-1	-1	-1	-1
$c_2(K=\pi)$	0.75	0.75	0.75	0.75	0.75
$c_3(K=\pi)$	0.3125	0.3125	0.3125	0.3125	0.3125
$c_4(K=\pi)$	-0.203125	-0.203125	-0.203125	-0.203125	-0.203125

Table V.1: Series coefficients of the two-triplon bound-state with total spin-0 and total momentum $K = \pi$ for different system sizes N.

N	10	20	30	40	50
$c_1(K=3\pi/4)$	-1.1464465	-1.1464466	-1.1464466	-1.1464466	-1.1464466
$c_2(K=3\pi/4)$	1.0991109	1.0991116	1.0991116	1.0991116	1.0991116
$c_3(K=3\pi/4)$	0.3585980	0.358589	0.358589	0.358589	0.358589
$c_4(K=3\pi/4)$	-0.3097861	-0.3097436	-0.3097436	-0.3097436	-0.3097436

Table V.2: Series coefficients of the two-triplon bound-state with total spin-0 and total momentum $K = 3\pi/4$ for different system sizes N.

V.1.1.2 Heisenberg ladder three-triplon bound-states

Next we want to discuss a scenario where this method fails. We will look at the three-triplon sector with total spin-0 as introduced in section IV.2.2. We established that in this first non-trivial order a bound-state exists only at total momentum $K = 0$ which is degenerate with the lower edge of the continuum. If we perform numerical diagonalisation on finite systems the energy gap between the bound-state and the

lowest energy quasi-free state is always finite thus non-degenerate perturbation theory is applicable. But unlike in the previous section this energy gap converges to zero as the system size N increases to the thermodynamic limit. Table V.3 shows the behaviour of the first four coefficients of the three-particle bound-state energy at total momentum $K = 0$ for different system sizes N. We notice that the coefficients for orders 3 and higher diverge as is expected due to the degeneracy with the continuum, as in these orders terms proportional to $1/(E_0 - E_i)$ appear. The Table also includes the expectation value for the sum of distances between the three particles which stays finite and does not scale proportional to the system size which indicates a bound-state as will be discussed in the following section V.2. Note that degenerate perturbation theory would be useless in this scenario since even if we considered the energetically next higher state to be degenerate with the bound-state the third lowest energy state would get arbitrarily close in energy to these states too. In the thermodynamic limit there is always an infinite amount of continuum states arbitrarily close to the bound-state disqualifying any finite dimensional degenerate perturbation theory.

N	10	15	20	25
D_Φ	2.63077	2.64563	2.65080	2.65414
$c_1(K=0)$	-1.49993938	-1.49999992	-1.50000000	-1.50000000
$c_2(K=0)$	1.56096097	1.55419467	1.55185257	1.55064888
$c_3(K=0)$	-1.86385	-4.44671×10^2	-1.63644×10^5	-8.12907×10^7
$c_4(K=0)$	1.65288×10^2	5.75787×10^6	8.05309×10^{11}	2.03389×10^{17}

Table V.3: Series coefficients of the three-triplon bound-state with total spin-0 and total momentum $K = 0$ for different system sizes N. Including the expectation value D_Φ for the sum of distances between the particles in the bound-state in first-non-trivial order.

V.2 Detecting bound-states via their distance expectation values

Often bound-states obtained from numerical diagonalisation are not easily identified via their energy gap to the continuum, especially if one works with small interaction strengths, where bound-states may or may not exist. A better ansatz analogous to methods used by Zhang, Braak and Kollar [18] is to look at the scaling behaviour of expectation values. We are specifically interested in the expectation values of the average distance between the particles. For a system of m particles, labelled by the basis states $|\boldsymbol{r}_1, \boldsymbol{r}_2, ..., \boldsymbol{r}_m\rangle$ with the n-th particle at lattice site $\boldsymbol{r}_n$, we define the operator $\widehat{d}_{ij}$ as

$$\widehat{d}_{ij} \left| \boldsymbol{r}_1, \boldsymbol{r}_2, ..., \boldsymbol{r}_m \right\rangle = \left| \boldsymbol{r}_i - \boldsymbol{r}_j \right| \left| \boldsymbol{r}_1, \boldsymbol{r}_2, ..., \boldsymbol{r}_m \right\rangle \ . \tag{V.9}$$

With this we define the sum of distance operator for m particles $\widehat{D}_m$ as

$$\widehat{D}_m = \sum_{i \neq j} \widehat{d}_{i,j} \ . \tag{V.10}$$

Let us now consider an m-particle bound state $\left| \Psi^{(m)}_{\text{Bound}}(N) \right\rangle$ and a m-particle quasi-free state $\left| \Psi^{(m)}_{\text{free}}(N) \right\rangle$ on a finite system with N sites in every independent direction given by the dimension d of the lattice. We consider the two expectation values of these states with regard to the average distance operator (V.10) as functions of the system size

$$\begin{aligned} D_{\text{Bound}}(N) &= \left\langle \Psi^{(m)}_{\text{Bound}}(N) \right| \widehat{D}_m \left| \Psi^{(m)}_{\text{Bound}}(N) \right\rangle \\ D_{\text{free}}(N) &= \left\langle \Psi^{(m)}_{\text{free}}(N) \right| \widehat{D}_m \left| \Psi^{(m)}_{\text{free}}(N) \right\rangle \ . \end{aligned} \tag{V.11}$$

Considering the scaling of these functions we expect that bound-states are localised in their relative distances and that the only N dependence in $D_{\text{Bound}}(N)$ arises due to finite size effects. Especially for large N we expect that the expectation value stays constant in N. In contrast a quasi-free state is a scattering state leading to no localisation in the particles' relative distances and thus we expect that for large N (ignoring finite size effects) the expectation value $D_{\text{free}}(N)$ scales like the average distance of m randomly placed points on a identical lattice of size N, which is usually proportional to N^1. We therefore expect

$$\begin{aligned} D_{\text{Bound}}(N) &\propto N^0 \\ D_{\text{free}}(N) &\propto N^1 \ . \end{aligned} \tag{V.12}$$

Note that this also holds if the quasi-free state contains bound-states of less than m particles. For example a three-particle scattering state of a two-particle bound state and a quasi-free single particle.
We can use this to find bound-states by plotting the average distance of all eigenstates $|\Phi\rangle$ that where numerically determined via ND against a list of the eigenstates (or their eigenenergies) for multiple system sizes N. While the bulk of states will scale linearly with the system size, the m-particle bound-states will remain at a constant (up to finite-size effects) value.

V.2.1 Examples

V.2.1.1 XXZ chain two-particle bound state

We will illustrate this technique with the known results for the XXZ model in the two-particle sector. Figure V.1 depicts the ND results of finite XXZ-models with periodic boundary conditions in the two-particle sector for different system sizes and a ratio $\lambda/J = 1/2$ for total momenta $K = \pi$ and $K = \pi/2$. For the ratio $\lambda/J = 1/2$ the bound-state exist only at total momenta which satisfy the inequality

$$\cos(K/2) < \frac{\lambda}{J} = \frac{1}{2} \,, \tag{V.13}$$

thus, as expected from the analytical results, only the right side of figure V.1 shows a bound-state, while the left side of figure V.1 depicts only quasi-free states.

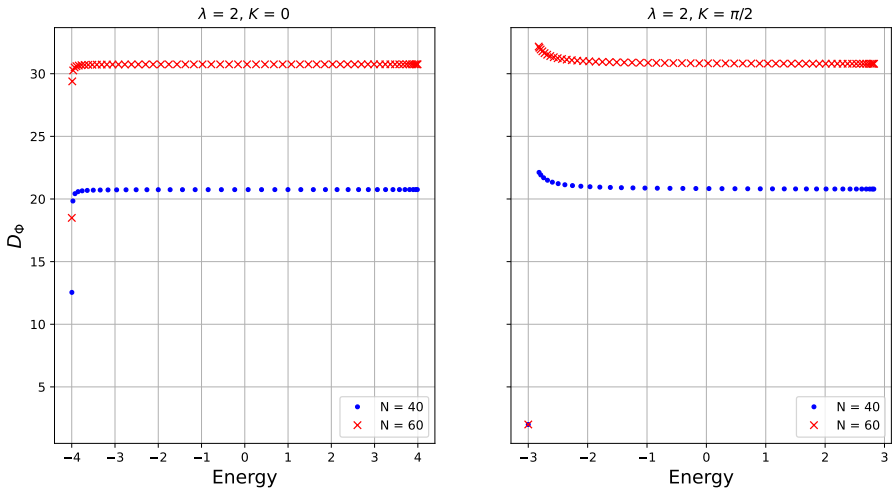

Figure V.1: Expectation value of the distance between two particles in the one-dimensional XXZ model for nearest-neighbour interaction strengths $\lambda/J = 2$ and $K = 0$ (left) and $K = \pi/2$ (right). Only the right figure displays a bound-state according to equation (IV.8).

V.2.1.2 XXZ chain three-particle bound states

Looking at the three-particle sector of the XXZ model we can show that this method is also capable to detect bound-states inside the continuum. To do so we note that at total momentum $K = 0$ the bound-state condition (IV.9) reduces to

$$0 < \left(\frac{\lambda}{J}\right)^2 , \tag{V.14}$$

i.e. it is always satisfied. Note that the energy of the bound-state is inside the continuum for $\frac{\lambda}{J} < 1$ and outside the continuum for $\frac{\lambda}{J} > 1$. Figures V.2 and V.3 depict these two cases with and without periodic boundary conditions respectively. Note that bound-states inside the continuum can only be seen with periodic boundary conditions.

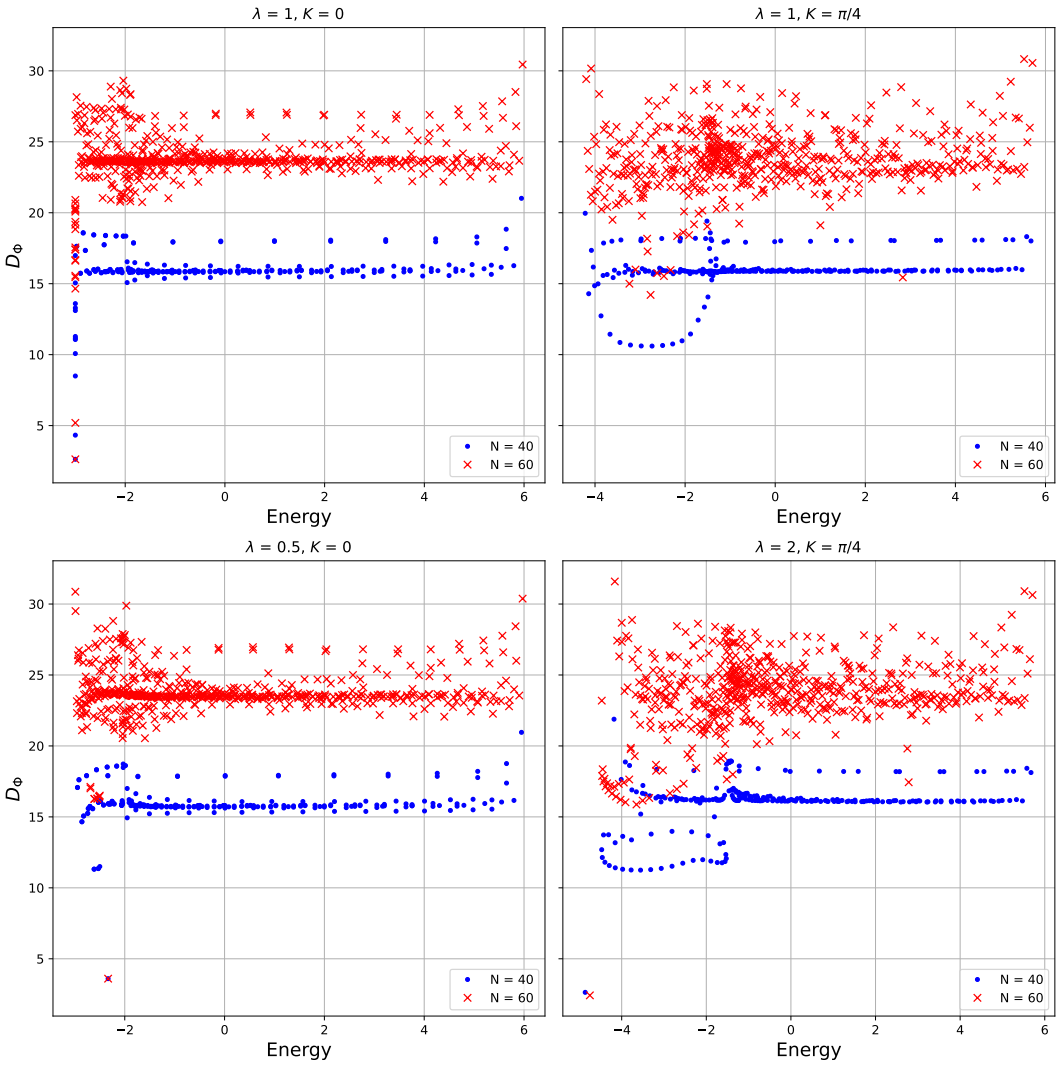

Figure V.2: Expectation value of the sum of distances D_ϕ between three particles in the one-dimensional XXZ model for different nearest-neighbour interaction strengths λ and total momenta K with periodic boundary conditions. For the cases $\lambda = 1$ and $\lambda = 0.5$ at total momentum $K = 0$ a bound-state can be seen.

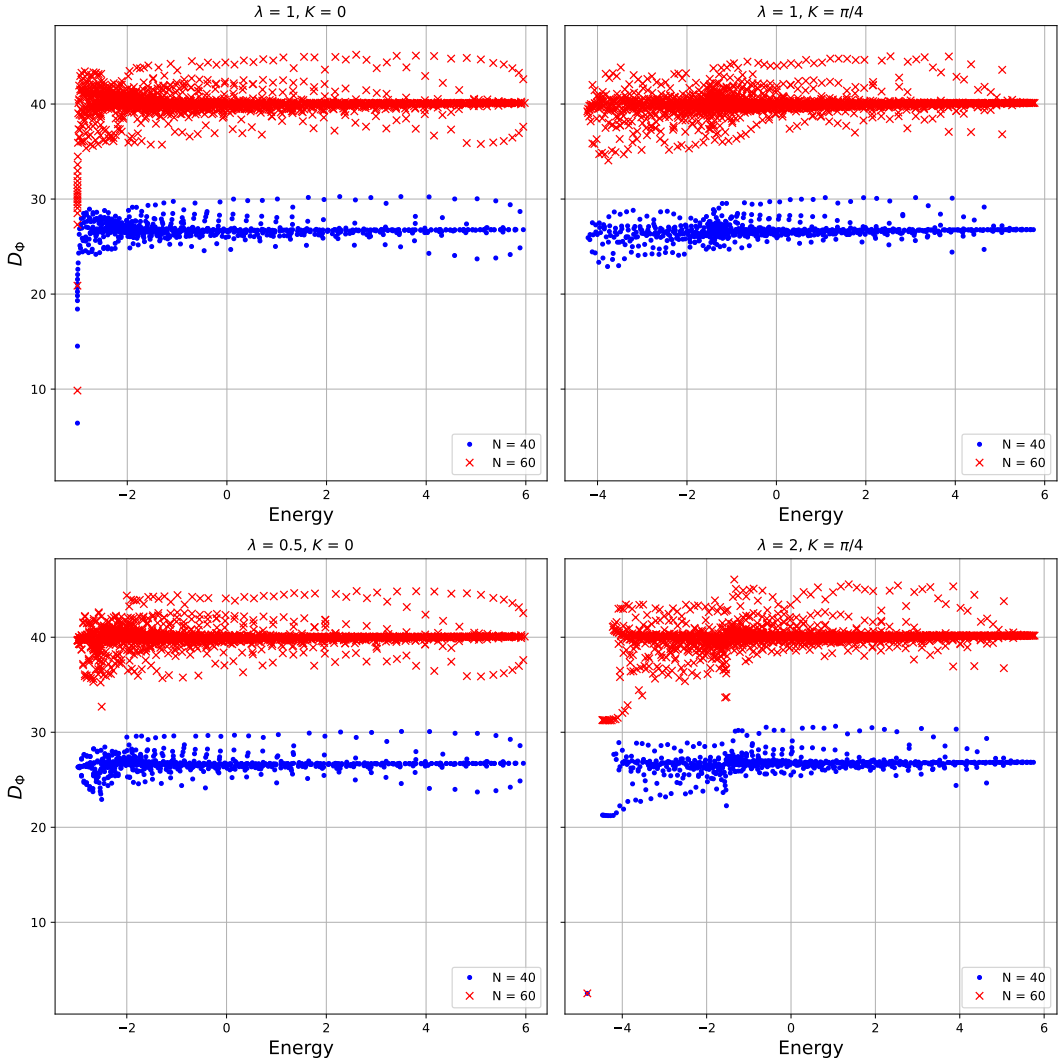

Figure V.3: Expectation value of the sum of distances D_ϕ between three particles in the one-dimensional XXZ model for different nearest-neighbour interaction strengths λ and total momenta K with non-periodic boundary conditions. The bound-state at $K = 0$ for $\lambda <= 1$ can no longer be detected, while the scaling of the bound-state at finite total momentum $K = \pi/4$ with $\lambda = 2$ is improved.

V.2.1.3 Heisenberg ladder three-triplon bound-states

As shown in section V.1.1.2 we are not able to obtain series expansions of the three-triplon bound-state using perturbation theory on ND results. Nevertheless we are able to detect the bound-state using the expectation value scaling technique. As in the previous case with the three-particle bound-states of the XXZ model inside the continuum, we are able to detect the three-triplon bound-state of the Heisenberg ladder in the total spin-0 sector at total momentum $K = 0$ in first-order at the lower edge of the continuum as shown in the previous example V.2. Including the second and third-order correction (only second-order corrections are necessary for this effect) to the effective Hamiltonian we find that at small values of the perturbation parameter $x = J_{\parallel}/J_{\perp}$ the bound-state exists at small values of the total momentum $K > 0$ (see figure V.4).

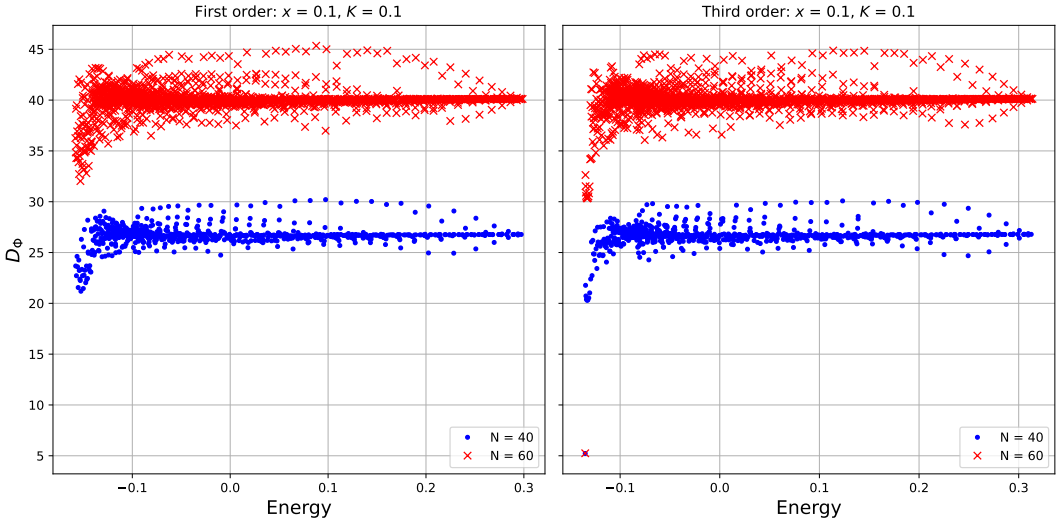

Figure V.4: Expectation value of the sum of distances between three particles in the Heisenberg ladder in first- and third-order at finite total momentum $K = 0.1$. The higher order terms of the model allow for a bound-state to form at total momenta other than $K = 0$. The boundary conditions are non-periodic.

VI Analytical methods for two-particle bound-state energies

VI.1 The Green's function method for bound-state energies

In this section we will discuss how two-particle bound-state energies can be obtained via the study of two-particle zero temperature Green's functions. This method is based on the Schmidt method in the study of integral equations [19] and is an application of the Dyson equation, similar techniques have been used in the context of quantum field theories [20] and the calculation of bound-states to impurities [21], while potential generalisations have been discussed by Faddeev [22], though not in the context of explicitly calculating bound-state energies. The aim of this chapter is the derivation of an implicit expression for these bound-state energies requiring only finite expressions, i.e., which only requires a finite dimensional matrix with matrix elements that demand at most the evaluation of integrals over the Brillouin zone.
We start from a Hamiltonian H that is particle number conserving. We are interested in the two-particle bound-state energies $\epsilon^{(2)}_{\text{Bound}}$ of this Hamiltonian, which have to be eigenvalues of H, i.e. there exists a state $|\Psi\rangle$ with

$$\begin{aligned} H\,|\Psi\rangle &= \epsilon^{(2)}_{\text{Bound}}\,|\Psi\rangle \\ Q\,|\Psi\rangle &= 2\,|\Psi\rangle \ , \end{aligned} \tag{VI.1}$$

where Q is the particle number operator. We can rewrite the eigenvalue equation as

$$\left(\epsilon^{(2)}_{\text{Bound}}\mathbb{1} - H\right)|\Psi\rangle = 0 \ . \tag{VI.2}$$

This just indicates that $|\Psi\rangle$ is part of the kernel of the operator $H - \epsilon_{\text{Bound}}\mathbb{1}$. We now define the zero temperature Green's function or resolvent of the operator H via

$$G(z) = (z\mathbb{1} - H)^{-1} \ . \tag{VI.3}$$

The main idea of this method relies on the fact that the resolvent does not formally exist, if z is an eigenvalue of H. We will use this property to search for eigenvalues

of H instead of trying to solve the eigenvalue equation directly. Note that the non-invertibility of the resolvent $G(z)$ is synonymous with the condition

$$\mathbf{det}\,(z\mathbb{1} - H) = 0 \tag{VI.4}$$

which of course is just the eigenvalue equation in the form of a characteristic polynomial. In the context of lattice models the Hamiltonian H is usually defined on an infinite lattice and the calculation of the characteristic polynomial is in most cases not directly feasible. We will use the properties of the zero temperature Green's function to reduce the calculation of the characteristic polynomial in the two-particle sector to the determinant of a finite matrix even for infinite systems, with a size only determined by the dimensionality and effective interaction range of the problem, which will become apparent in the following section.

VI.1.1 Implicit eigenvalue equations

For our general setup we will assume a particle number conserving Hamiltonian H translationally invariant defined on a lattice with sites $i \in L$ and an assortment of a finite number of distinct local bosons described by their creation- and annihilation operators $b^\dagger_{\alpha,i}$, $b_{\alpha,i}$ where the index α denotes the kind of boson and i denotes the lattice site the boson is created/ destroyed on. We will assume H to be normal ordered. A description in terms of fermions or a mixture of bosons and fermions is analogous to the method described below for bosons. A hard-core bosonic problem can be mapped onto the bosonic case as will be discussed in chapter VI.1.6. We will therefore restrict our attention to the purely bosonic case.
Due to the particle number conservation of the Hamiltonian H we may split it into a free H_0 and interacting part V

$$H = H_0 + V\ , \tag{VI.5}$$

where H_0 and V are solely defined by the number of creation and annihilation operators they contain. H_0 will be quadratic in the number of creation and annihilation operators

$$H_0 = \sum_{\alpha,\beta} \sum_{\boldsymbol{i},\boldsymbol{j}\in L} J^{\alpha,\beta}_{\boldsymbol{i},\boldsymbol{j}} b^\dagger_{\alpha,\boldsymbol{i}} b_{\beta,\boldsymbol{j}} \tag{VI.6}$$

while V will be quartic in the number of creation and annihilation operators

$$V = \sum_{\alpha,\beta,\gamma,\omega} \sum_{\boldsymbol{i},\boldsymbol{j},\boldsymbol{m},\boldsymbol{n}\in L} J^{\alpha,\beta,\gamma,\omega}_{\boldsymbol{i},\boldsymbol{j},\boldsymbol{m},\boldsymbol{n}} b^\dagger_{\alpha,\boldsymbol{i}} b^\dagger_{\beta,\boldsymbol{j}} b_{\gamma,\boldsymbol{m}} b_{\omega,\boldsymbol{n}}\ . \tag{VI.7}$$

Terms proportional to the identity are neglected here, as they only shift all energies. In the following we will set the ground-state energy equal to zero and look at all energies relative to the ground-state energy instead. In practice this split can be systematically performed by calculating the irreducible one-particle matrix elements to obtain H_0 and the irreducible two-particle elements for V, following the methods discussed in chapter III.2.4.
Next, we will rewrite the eigenvalue equation in form of the characteristic polynomial (VI.4) using the free and interacting part as

$$\begin{aligned}\mathbf{det}\left(z\mathbb{1}-H\right) &= \mathbf{det}\left(z\mathbb{1}-H_0-V\right)\\ &= \mathbf{det}\left(\left(z\mathbb{1}-H_0\right)\left(\mathbb{1}-\left(z\mathbb{1}-H_0\right)^{-1}V\right)\right)\\ &= \mathbf{det}\left(z\mathbb{1}-H_0\right)\,\mathbf{det}\left(\mathbb{1}-\left(z\mathbb{1}-H_0\right)^{-1}V\right)\\ &= \mathbf{det}\left(z\mathbb{1}-H_0\right)\,\mathbf{det}\left(\mathbb{1}-G_0(z)V\right)\,,\end{aligned} \tag{VI.8}$$

where we defined the zero temperature Green's function of the free Hamiltonian H_0 as $G_0(z) = (z\mathbb{1} - H_0)^{-1}$. This formula is just an example of the second resolvent identity. As discussed previously, a two-particle spectrum consists of a two-particle continuum and potential bound-states outside this continuum (exceptions to this exist in integrable models, where bound-states can also be present inside the continuum, which will not be considered here). The two-particle continuum at a given total momentum K of two particles can be obtained by taking all sums of one-particle energies $\omega(k)$, i.e. $\{\omega(k)+\omega(K-k)\}_{k\in 1.\mathrm{B.Z.}}$, over the entire first Brillouin zone (1. B.Z.). By Weyl's theorem [6] this spectrum is independent of compact perturbations. In our context this means that the two-particle spectrum is fully described by H_0 if for a given total momentum the interaction part V is compact which is always the case if it is of finite range.
Therefore all eigenvalues of H_0 in the two-particle sector lie in the two-particle continuum, i.e. we know that

$$\mathbf{det}\left(z\mathbb{1}-H_0\right) \neq 0 \tag{VI.9}$$

for z outside the two-particle continuum. Looking for two-particle bound-states we can therefore restrict our attention to the equation

$$\mathbf{det}\left(\mathbb{1}-G_0(z)V\right) = 0 \tag{VI.10}$$

noting that this equation is only well defined outside the continuum for real values of z.

This is the equation we want to use to determine the two-particle bound-state energies, by reducing it to the determinant of a finite matrix. We can do this by defining a projection operator P such that it projects on the smallest subspace where the interaction V acts different from the zero operator

$$PV = VP = V \ . \tag{VI.11}$$

Thus we can rewrite the implicit eigenvalue equation (VI.10) as

$$\mathbf{det}\left(\mathbb{1} - G_0(z)VP\right) = 0 \tag{VI.12}$$

which after applying the Weinstein-Aronszajn identity for determinants yields

$$\mathbf{det}\left(\mathbb{1} - PG_0(z)V\right) = 0 \ . \tag{VI.13}$$

Note that the projection operator is not necessary for the following argument but is a good reminder for the block diagonal form of the new matrix $\mathbb{1} - PG_0(z)V$. This new matrix is only different from the identity matrix on the subspace where V acts different from the zero operator. The matrix therefore assumes a block-diagonal form and as such its determinant can be restricted to this subspace. This equation is the backbone of this method as it allows us to reduce any two-particle bound-state problem on a lattice with finite range interaction and translational invariance to the determinant of a finite matrix and an implicit equation similar to the characteristic polynomial.

VI.1.2 Explicit form of the implicit equation

We want to give explicit expressions for the implicit equation determining the energy of a bound state (VI.13) by choosing two specific basis sets for the general problem. First, we will look at the free Hamiltonian

$$H_0 = \sum_{\alpha,\beta} \sum_{\boldsymbol{i},\boldsymbol{j} \in L} J_{\boldsymbol{i},\boldsymbol{j}}^{\alpha,\beta} b_{\alpha,\boldsymbol{i}}^\dagger b_{\beta,\boldsymbol{j}} \ . \tag{VI.14}$$

Free bosons can always be diagonalised via a Fourier transformation and a diagonalisation inside the unit cell. We introduce the Fourier transformation

$$\begin{aligned} b_{\alpha,\boldsymbol{k}}^\dagger &= \frac{1}{\sqrt{N}} \sum_{\boldsymbol{j} \in L} e^{\mathrm{i}\boldsymbol{j}\boldsymbol{k}} b_{\alpha,\boldsymbol{j}}^\dagger \\ b_{\alpha,\boldsymbol{k}} &= \frac{1}{\sqrt{N}} \sum_{\boldsymbol{j} \in L} e^{-\mathrm{i}\boldsymbol{j}\boldsymbol{k}} b_{\alpha,\boldsymbol{j}} \end{aligned} \tag{VI.15}$$

as well as a flavour mixing matrix M to define the new bosonic creation operators

$$\tilde{b}^\dagger_{\alpha,\boldsymbol{k}} = \sum_\beta M_{\alpha\beta} b^\dagger_{\beta,\boldsymbol{k}} \tag{VI.16}$$

such that H_0 is diagonal

$$H_0 = \sum_{\boldsymbol{k}} \sum_\alpha \omega_\alpha(\boldsymbol{k}) \tilde{b}^\dagger_{\alpha,\boldsymbol{k}} \tilde{b}_{\alpha,\boldsymbol{k}} \tag{VI.17}$$

where $\omega_\alpha(k)$ are the one-particle dispersions of the free system. With this we define the Fourier-basis

$$|\boldsymbol{k_1}, \boldsymbol{k_2}; \alpha, \beta\rangle = \sqrt{\frac{2 - \delta_{\boldsymbol{k_1},\boldsymbol{k_2}}\delta_{\alpha,\beta}}{2}} \tilde{b}^\dagger_{\alpha,\boldsymbol{k_1}} \tilde{b}^\dagger_{\beta,\boldsymbol{k_2}} |0\rangle \ . \tag{VI.18}$$

Here $|0\rangle$ is the state with 0 bosons and the prefactor is for normalisation, if two identical bosons are present.
This Fourier basis diagonalises the free Hamiltonian H_0 in the two-particle sector

$$H_0 |\boldsymbol{k_1}, \boldsymbol{k_2}; \alpha, \beta\rangle = (\omega_\alpha(\boldsymbol{k_1}) + \omega_\beta(\boldsymbol{k_2})) |\boldsymbol{k_1}, \boldsymbol{k_2}; \alpha, \beta\rangle \tag{VI.19}$$

allowing us to give an explicit expression for the zero-temperature Green's function of the free Hamiltonian in the two-particle sector

$$G_0(z) = (z\mathbb{1} - H_0)^{-1} = \sum_{\boldsymbol{k_1},\boldsymbol{k_2}} \sum_{\alpha,\beta} \frac{1 + \delta_{\boldsymbol{k_1},\boldsymbol{k_2}}\delta_{\alpha,\beta}}{2} \frac{|\boldsymbol{k_1}, \boldsymbol{k_2}; \alpha, \beta\rangle \langle \boldsymbol{k_1}, \boldsymbol{k_2}; \alpha, \beta|}{z - (\omega_\alpha(\boldsymbol{k_1}) + \omega_\beta(\boldsymbol{k_2}))} \ . \tag{VI.20}$$

Note that the additional factor in the sum is introduced to avoid double counting as the two particles are identical and $|\boldsymbol{k_1}, \boldsymbol{k_2}; \alpha, \beta\rangle = |\boldsymbol{k_2}, \boldsymbol{k_1}; \beta, \alpha\rangle$.
Next we take a look at the interaction operator V. In most systems the interaction between two particles is limited to the case where these two particles are at most d_c sites apart. To better capture this behaviour we introduce the bosonic (K,d)-basis

$$|\boldsymbol{K}; \boldsymbol{d}; \alpha, \beta\rangle = \sqrt{\frac{2 - \delta_{\boldsymbol{d},\boldsymbol{0}}\delta_{\alpha,\beta}}{2}} \frac{1}{\sqrt{N}} \sum_{\boldsymbol{j}} e^{\mathrm{i}\boldsymbol{j}\boldsymbol{K}} |\boldsymbol{j}, \boldsymbol{j} + \boldsymbol{d}; \alpha, \beta\rangle \tag{VI.21}$$

with $|\boldsymbol{j}, \boldsymbol{j} + \boldsymbol{d}; \alpha, \beta\rangle = b^\dagger_{\alpha,\boldsymbol{j}} b^\dagger_{\beta,\boldsymbol{j}+\boldsymbol{d}} |0\rangle$. Here $\boldsymbol{K}$ labels the total momentum of the two particles and $\boldsymbol{d}$ is the relative distance between them. The prefactor is again for

normalisation in the case that two identical particles are at the same site.
Our interaction is compact in the subspace with fixed total momentum $\boldsymbol{K}$ if there exist a value $d_c \geq 0$ such that

$$V \left|\boldsymbol{K}; \boldsymbol{d}; \alpha, \beta\right\rangle = 0 \tag{VI.22}$$

for all $|\boldsymbol{d}| > d_c$. The (K,d)-basis is often the simplest choice to calculate matrix elements of the matrix $G_0(z)V$, as the finite subspace is simply implemented by the constraint that $|\boldsymbol{d}| \leq d_c$. We only need the matrix elements of $G_0(z)$ in the (K,d)-basis. First, using the definitions of the Fourier- and (K,d)-basis (VI.18) and (VI.21), we calculate the overlap between two basis vectors

$$\begin{aligned}\left\langle \boldsymbol{k_1}, \boldsymbol{k_2}; \tilde{\alpha}, \tilde{\beta} \middle| \boldsymbol{K}; \boldsymbol{d}; \alpha, \beta \right\rangle = \delta_{\boldsymbol{K}, \boldsymbol{k_1}+\boldsymbol{k_2}} \sqrt{\frac{2 - \delta_{\boldsymbol{k_1},\boldsymbol{k_2}}\delta_{\alpha,\beta}}{2}} \sqrt{\frac{2 - \delta_{\boldsymbol{d},\boldsymbol{0}}\delta_{\alpha,\beta}}{2}} \\ \times \frac{1}{\sqrt{N}} \left(M^\dagger_{\tilde{\alpha},\beta} M^\dagger_{\tilde{\beta},\alpha} e^{-\mathrm{i}\boldsymbol{d}\boldsymbol{k_1}} + M^\dagger_{\tilde{\alpha},\alpha} M^\dagger_{\tilde{\beta},\beta} e^{-\mathrm{i}\boldsymbol{d}\boldsymbol{k_2}} \right) .\end{aligned} \tag{VI.23}$$

We can use this to calculate the matrix element

$$\begin{aligned}\langle \boldsymbol{K}; \boldsymbol{d_1}; \alpha, \beta | \, G_0(z) \, | \boldsymbol{K}, \boldsymbol{d_2}; \alpha', \beta' \rangle = \sqrt{\frac{2 - \delta_{\boldsymbol{d_1},\boldsymbol{0}}\delta_{\alpha,\beta}}{2}} \sqrt{\frac{2 - \delta_{\boldsymbol{d_2},\boldsymbol{0}}\delta_{\alpha',\beta'}}{2}} e^{\mathrm{i}(\boldsymbol{d_1}-\boldsymbol{d_2})\boldsymbol{K}/2} \\ \times \sum_{\tilde{\alpha},\tilde{\beta}} M_{\alpha,\tilde{\alpha}} M_{\beta,\tilde{\beta}} I^{(1)}_{\boldsymbol{d_1},\boldsymbol{d_2};\tilde{\alpha},\tilde{\beta}}(z;\boldsymbol{K}) M^\dagger_{\tilde{\alpha},\alpha'} M^\dagger_{\tilde{\beta},\beta'} + M_{\alpha,\tilde{\alpha}} M_{\beta,\tilde{\beta}} I^{(2)}_{\boldsymbol{d_1},\boldsymbol{d_2};\tilde{\alpha},\tilde{\beta}}(z;\boldsymbol{K}) M^\dagger_{\tilde{\alpha},\beta'} M^\dagger_{\tilde{\beta},\alpha'}\end{aligned} \tag{VI.24}$$

with the two real integrals

$$\begin{aligned} I^{(1)}_{\boldsymbol{d_1},\boldsymbol{d_2};\tilde{\alpha},\tilde{\beta}}(z;\boldsymbol{K}) &= \frac{1}{A_{\text{1.B.Z.}}} \int_{\text{1.B.Z.}} \frac{\cos\left((\boldsymbol{d_1} - \boldsymbol{d_2})\left(\boldsymbol{K}/2 - \boldsymbol{k}\right)\right)}{z - \left(\omega_{\tilde{\alpha}}(\boldsymbol{k}) + \omega_{\tilde{\beta}}(\boldsymbol{K} - \boldsymbol{k})\right)} d\boldsymbol{k} \\ I^{(2)}_{\boldsymbol{d_1},\boldsymbol{d_2};\tilde{\alpha},\tilde{\beta}}(z;\boldsymbol{K}) &= \frac{1}{A_{\text{1.B.Z.}}} \int_{\text{1.B.Z.}} \frac{\cos\left((\boldsymbol{d_1} + \boldsymbol{d_2})\left(\boldsymbol{K}/2 - \boldsymbol{k}\right)\right)}{z - \left(\omega_{\tilde{\alpha}}(\boldsymbol{k}) + \omega_{\tilde{\beta}}(\boldsymbol{K} - \boldsymbol{k})\right)} d\boldsymbol{k} \ , \end{aligned} \tag{VI.25}$$

where 1.B.Z. denotes the first Brillouin zone of the lattice and $A_{\text{1.B.Z.}}$ is the area of this first Brillouin zone. In the special case where only one particle flavour is present the flavour mixing matrices $M_{\alpha,\beta}$ are simply $M = 1$ and the real integral can be combined to

$$I_{\boldsymbol{d_1},\boldsymbol{d_2}}(z;\boldsymbol{K}) = I^{(1)}_{\boldsymbol{d_1},\boldsymbol{d_2}}(z;\boldsymbol{K}) + I^{(2)}_{\boldsymbol{d_1},\boldsymbol{d_2}}(z;\boldsymbol{K}) = \\ = \frac{2}{A_{\text{1.B.Z.}}} \int_{\text{1.B.Z.}} \frac{\cos\left(\boldsymbol{d_1}\left(\boldsymbol{K}/2-\boldsymbol{k}\right)\right)\cos\left(\boldsymbol{d_2}\left(\boldsymbol{K}/2-\boldsymbol{k}\right)\right)}{z-\left(\omega(\boldsymbol{k})+\omega(\boldsymbol{K}-\boldsymbol{k})\right)} d\boldsymbol{k} \ . \tag{VI.26}$$

These results allow us to directly compute the matrix elements of $G_0(z)$ in the (K,d)-basis. This is useful as in this basis only the finitely many matrix elements with $|\boldsymbol{d}| < d_c$ contribute to the determinant of the matrix $\mathbb{1} - PG_0(z)V$. By calculating this matrix in the (K,d)-basis with the above formulas we have thus managed to reduce the implicit equation (VI.13) to an equation involving only a finite matrix with known matrix elements, requiring only integrals over the first Brillouin zone.

VI.1.3 Calculation of two-particle bound-state energy series

As previously discussed a series expansion for a bound-state at total momentum K in a perturbation parameter x coming from a phase of free particles does not always exist in the form

$$\epsilon^{(2)}_{\text{Bound}}(K) = \epsilon_0(K) + \epsilon_1(K)x + \epsilon_2(K)x^2 + \dots \ . \tag{VI.27}$$

The Green's function method provides a way to calculate this series expansion if it does exist for two-particle bound-states but also enables an alternative to this approach yielding a systematic series expansion from with the bound-state energy can be derived implicitly.
We start from a perturbative Hamiltonian in the two QP-sector that can be split in the free hopping Hamiltonian H_0 and the interaction Hamiltonian V (here V includes the correction due to the hard-core to boson mapping described in section VI.1.6 if necessary). We can then perform the Green's function method and obtain our implicit expression for the bound state energy

$$\mathbf{det}\left(1 - PG_0(z,x,K)V(x,K)\right) = 0 \ . \tag{VI.28}$$

Our goal is to expand the left hand side of this equation into a power series in the perturbation parameter x. This is done in three steps:
First, we expand the interaction matrix $V(x,K)$. Starting from an effective Hamiltonian given in orders of x, this matrix is usually already given as a power series in x up to a given order so nothing further has to be done.
Second, we expand the Green's function $G_0(z,x,K)$. Its dependence on x arises due to the one-particle dispersion

$$\omega(x,k) = \omega_0(k) + \omega_1(k)x + \omega_2(k)x^2 + ... \ , \tag{VI.29}$$

where the prefactors are sums of cosine and sine functions in the one-particle momentum k. A given entry of the Green's function matrix is then of the form

$$\begin{aligned}(G_0(z,x,K))_{d,d'} &= \frac{1}{A_{\text{1.B.Z.}}} \int_{\text{1.B.Z.}} \frac{f_{d,d'}(k,K)}{z-(\omega(x,k)+\omega(x,K-k))} d^n k = \\ &= \frac{1}{A_{\text{1.B.Z.}}} \sum_{m=0}^{\infty} \int_{\text{1.B.Z.}} f_{d,d'}(k,K) \frac{(\omega(x,k)-\omega_0(k)+\omega(x,K-k)-\omega_0(K-k))^m}{(z-(\omega_0(k)+\omega_0(K-k)))^{m+1}} d^n k\end{aligned} \tag{VI.30}$$

where we expanded the fraction as a geometric series. If we choose z outside the zeroth-order two-particle continuum at $x = 0$ given by the set $\text{Imag}\,(\omega_0(k_1) + \omega_0(k_2))$, we ensure that $z - (\omega_0(k) + \omega_0(K-k)) \neq 0$ and thus a non-zero range around $x = 0$ exists for which this geometric series converges.
Notice that each summand in the sum indexed by m now contains a term $\omega(x,k) - \omega_0(k) \propto x$ and higher orders in x. Thus if we desire an expansion in x up to some finite order M (usually the order of the effective Hamiltonian we started with), we can just replace the sum

$$\sum_{m=0}^{\infty} \to \sum_{m=0}^{M} \ . \tag{VI.31}$$

If multiple particle flavours are present, the functions $f_{d,d'}(k,K)$ contain the flavour mixing matrices $M_{\alpha,\beta}$ which can be dependent on the perturbation parameter. These can be expanded in orders of the perturbation parameter using regular potentially degenerate perturbation theory on the flavour subspace. We can thus write the matrix element in the form

$$(G_0(z,x,K))_{d,d'} = g^{(0)}_{d,d'}(z,K) + g^{(1)}_{d,d'}(z,K)x + g^{(2)}_{d,d'}(z,K)x^2 + O(x^{M+1}) \tag{VI.32}$$

where $g^{(0)}_{d,d'}(z,K) = (G_0(z,0,K))_{d,d'}$.
The third step consists of evaluating the determinant. Using the previous steps, the matrix $1 - PG_0(z,x,K)V(x,K)$ can be expressed as a power series in x up to a desired order and the determinant thus also yields a polynomial in these quantities.
We end up with an expression of the form

$$\textbf{det}\ (1 - PG_0(z,x,K)V(x,K)) = f(z,x,K) = \sum_{m=0}^{M} f_m(z,K)x^m + O\left(x^{M+1}\right) \quad \text{(VI.33)}$$

up to some order M.
A series expansion for a bound-state energy $\epsilon^{(2)}_{\text{Bound}}(x)$ can now be obtained by putting the ansatz (VI.27) into the function $f(z,x,K)$ and again expanding in orders of x

$$f(\epsilon^{(2)}_{\text{Bound}}(x),x,K) = \tilde{f}_0(\epsilon_0) + \tilde{f}_1(\epsilon_0,\epsilon_1)x + \tilde{f}_2(\epsilon_0,\epsilon_1,\epsilon_2)x^2 + \dots\ . \quad \text{(VI.34)}$$

Notice that the $m-$th coefficient of f only depends on the coefficients of the bound-state energy up to order m. We can thus solve the equation

$$f(\epsilon_{\text{Bound}}(x),x,K) = 0 \quad \text{(VI.35)}$$

recursively order by order to obtain an expansion for the bound-state energy. Note that the coefficient ϵ_m only appears linearly in the coefficient $\tilde{f}_m$, therefore only simple linear equations have to be solved in this recursive process. The only exception is the first coefficient $\tilde{f}_0(\epsilon_0)$. This is in general a non-trivial function of the bound-state energy ϵ_0 and has to be solved numerically for every value of the total momentum K. Also note that in the cases, where no bound-state exists at $x = 0$, the equation $\tilde{f}_0(\epsilon_0) = 0$ will have no solution outside the zeroth-order two-particle continuum.
In this case, where no bound-state exists at $x = 0$, i.e. $\tilde{f}_0(\epsilon_0) \neq 0$ for all choices of ϵ_0 outside the two-particle continuum, we can still calculate the implicit function as a power series (VI.33). This series can not only be used to determine the energy implicitly but can also be used to extrapolate the calculation to larger values of x, by employing series extrapolation methods like Padé-expansions. This is often even necessary to obtain reasonable results from these series in some finite order, as the original functions they approximate usually have a pole at the the edges of the zeroth-order two-particle continuum, if a bound-state is present, as seen in the examples below VI.1.7.

VI.1.4 Calculating the two-particle gap and critical exponents

In the previous section the implicit function $f(z,x,K)$ was introduced as a method to determine the energy of two-particle bound-states. We can also use this function to study quantum phase transitions in a scenario where the two-particle gap $\Delta^{(2)}$, that is the smallest energy gap between a two-particle bound-state and the ground-state, closes before the one-particle energy gap $\Delta^{(1)}$.

First some words of clarification. The distinction between a one- and two-particle energy gap is artificial in the sense that a second order quantum phase transition is driven by the closing of the gap between the ground-state and its lowest excitation. The distinction between different gaps only arises if we study the quantum phase transition from a point in parameter space far away from it, where we initially introduce the notion of conserved quasi-particles. When we then get closer to the quantum phase transition these particles that where introduced in a different regime of the parameter space need no longer describe the energy hierarchies (i.e. the ordering that $(n+1)$-particle states have higher energies than n-particle states) close to the quantum phase transition.
A more practical problem arising with the ansatz of studying a quantum phase transition, using an effective Hamiltonian starting from a point in parameter space that is adiabatically connected but can be far away from the quantum phase transition, are questions of convergence. Usually any perturbative approximation of the true Hamiltonian breaks down as one approaches the quantum phase transition, as a perturbative approximation can not capture the behaviour right at or beyond this point. Thus one employs extrapolation techniques in the study of these quantum phase transitions. In the case of the one-particle gap we can use the effective Hamiltonian to derive exact series expansions for the ground-state energy and one-particle dispersion of the system which lead to an exact series expansion of the one-particle energy gap. This series expansion can then be extrapolated using techniques like Padé- or DlogPadé-approximations [17] to obtain the behaviour of the gap close to the quantum phase transition. Unfortunately in the case of two-particle bound-state energies often no series expansion around the initial limit exists as discussed in previous chapters (see V and VI.1.3) thus different ways to extrapolate the gap have to be applied.
The implicit function $f(z,x,K) = \mathbf{det}\,(1 - PG_0(z,x,K)V(x,K))$ contains all necessary information about the two-particle bound-state energy and can be expanded in a series around the initial limit $x = 0$ as seen in the previous chapter VI.1.3. To obtain the gap and the critical exponents we make the following observations.
The function $f(z,x,K)$ is a holomorphic function in the z-argument, thus we can expand it as

$$f(z,x,K) = f_0(x,K) + f_1(x,K)(z_0 - z) + O((z_0 - z)^2)\ . \tag{VI.36}$$

We further know that the two-particle bound-state energy $\epsilon^{(2)}_{\text{Bound}}(x,K)$ is a root of $f(z,x,K)$ in the z-argument

$$f(\epsilon^{(2)}_{\text{Bound}}(x,K),x,K) = 0\ . \tag{VI.37}$$

Thus, by choosing $z_0 = \epsilon^{(2)}_{\text{Bound}}(x,K)$ we find

$$f(z,x,K) = f_1(x,K)(\epsilon^{(2)}_{\text{Bound}}(x,K) - z) + O((\epsilon^{(2)}_{\text{Bound}}(x,K) - z)^2) \ . \tag{VI.38}$$

If we now assume that the quantum phase transition is driven by the closing of the two-particle gap we find that by evaluating $f(z,x,K)$ at $z = \epsilon_{\text{ground}}(x)$ with the ground-state energy $\epsilon_{\text{ground}}(x)$ a function of the perturbation parameter x is obtained which is zero exactly at the critical value x_{crit} at which the two-particle gap $\Delta^{(2)}(x,K)$ at a specific total momentum K closes, i.e.

$$\tilde{f}(x,K) = f(z = \epsilon_{\text{ground}}(x), x, K) = f_1(x,K)\Delta^{(2)}(x,K) + O((\Delta^{(2)}(x,K))^2) \tag{VI.39}$$

with $\epsilon^{(2)}_{\text{Bound}}(x,K) - \epsilon_{\text{ground}}(x) = \Delta^{(2)}(x,K)$. We notice that the function $\tilde{f}(x,K)$ is not equivalent or simply proportional to the two-particle bound-state energy gap $\Delta^{(2)}(x,K)$, but it can be expressed as a series expansion around $x = 0$ as discussed in the previous chapter (we assume that a series expansion for the ground-state energy $\epsilon_{\text{ground}}(x)$ is known here). This is notable as $\Delta^{(2)}(x,K)$ does often not posses a series expansion around $x = 0$ as discussed in the previous chapter V.
Following our previous assumption that the quantum phase transition is driven by the closing of the two-particle bound-state energy gap $\Delta^{(2)}(x,K_{\text{crit}})$ at some specific value of the total momentum K_{crit} we use the power-law behaviour [5]

$$\Delta^{(2)}(x,K_{\text{crit}}) \propto |x - x_{\text{crit}}|^{z\nu} \tag{VI.40}$$

for parameters x close to the critical value x_{crit}, with the critical exponents z and ν. If we now assume that the prefactor function $f_1(x,K_{\text{crit}})$ approaches a constant non-zero value as the parameter x gets close to the value of the quantum phase transition, i.e. $\lim_{x\to x_{\text{crit}}} f_1(x,K_{\text{crit}}) = c \neq 0$ we find

$$\tilde{f}(x,K_{\text{crit}}) \propto |x - x_{\text{crit}}|^{z\nu} + O(|x - x_{\text{crit}}|^E) \tag{VI.41}$$

with corrections of orders E larger than $z\nu$.
To summarise, using the implicit function $f(z,x,K)$ obtained via the Green's function method, we are able to derive a series expansion for the function $\tilde{f}(x,K_{\text{crit}})$ around the initial limit $x = 0$. This function $\tilde{f}(x,K_{\text{crit}})$ can be shown to have a leading order behaviour identical to the gap of a system whose quantum phase transition is characterised by the closing of a two-particle bound-state energy gap. Using this we can extract the critical point x_{crit} and the critical exponent $z\nu$ from the series expansion of $\tilde{f}(x,K_{\text{crit}})$ using techniques like DlogPadé [17] without the necessity for a series expansion of the two-particle bound-state energy around the initial limit $x = 0$ which usually does not exist.

VI.1.5 Problems arising in the three and higher particle sectors

We want to discuss the limitations of this method for studying bound-states containing more than two particles. The ability to reduce the eigenvalue equation to a equation containing only the determinant of a finite matrix relies on the finite dimensional image of the interaction operator on a given total momentum subspace in the two-particle sector. This no longer holds for two-particle interactions with finite range in the three-particle sector as now any state with two-particles close enough to each other is outside the kernel of the interaction operator no matter how far away the third particle is from them (analogously for any other particle sector larger than two). While the above equations still hold in these higher particle sectors the determinant in the pivotal equation (VI.13) can no longer be reduced to the determinant on a finite subspace. For completeness and to further discuss this point we will derive an analogous equation to (VI.13) based on methods developed by Faddeev [22] for the three-particle sector. We start with a Hamiltonian containing two-particle $V^{(2)}$ and three-particle interactions $V^{(3)}$

$$H = H_0 + V^{(2)} + V^{(3)} = H_0 + V \ . \tag{VI.42}$$

We use the resolvent equations

$$\begin{aligned} G(z) &= (z - H)^{-1} = G_0 + G_0 V G = G_0 + G_0 T(z) G_0 \\ T(z) &= V + V G_0 T(z) \end{aligned} \tag{VI.43}$$

and define the pure two-/ three-particle T-operators

$$\begin{aligned} T^{(2)}(z) &= V^{(2)} + V^{(2)} G_0 T^{(2)}(z) \\ T^{(3)}(z) &= V^{(3)} + V^{(3)} G_0 T^{(3)}(z) \ . \end{aligned} \tag{VI.44}$$

Similar to Faddeev's method we define two new T-operators

$$\begin{aligned} T_2(z) &= V^{(2)} + V^{(2)} G_0 T(z) \\ T_3(z) &= V^{(3)} + V^{(3)} G_0 T(z) \end{aligned} \tag{VI.45}$$

where $T(z)$ is the T-operator with respect to the full interaction $V = V^{(2)} + V^{(3)}$. With this we immediately find

$$T(z) = V + VG_0T(z) = T_2(z) + T_3(z) \ . \tag{VI.46}$$

We will quickly derive a general equation assuming an interaction of the form $V = \sum_i V^{(i)}$ and the T-operators $T^{(i)}$ and T_i defined as above. We find

$$\begin{aligned} T_j &= V^{(j)} + V^{(j)}G_0 \sum_i T_i \\ \left(1 - V^{(j)}G_0\right) T_j &= V^{(j)} + V^{(j)}G_0 \sum_{i\neq j} T_i \\ T_j &= T^{(j)} + T^{(j)}G_0 \sum_{i\neq j} T_i \end{aligned} \tag{VI.47}$$

where we used that $T^{(j)} = \left(1 - V^{(j)}G_0\right)^{-1} V^{(j)}$. These equations can be written in matrix form with operators as their entries. In the case of the three-particle problem with the interaction $V = V^{(2)} + V^{(3)}$ as defined above, we find

$$\begin{pmatrix} T_2 \\ T_3 \end{pmatrix} = \begin{pmatrix} T^{(2)} \\ T^{(3)} \end{pmatrix} + \begin{pmatrix} 0 & T^{(2)}G_0 \\ T^{(3)}G_0 & 0 \end{pmatrix} \begin{pmatrix} T_2 \\ T_3 \end{pmatrix} \ . \tag{VI.48}$$

Neglecting questions of convergence we rewrite this as an infinite series of the form

$$\begin{pmatrix} T_2 \\ T_3 \end{pmatrix} = \sum_{n=0}^{\infty} \begin{pmatrix} 0 & T^{(2)}G_0 \\ T^{(3)}G_0 & 0 \end{pmatrix}^n \begin{pmatrix} T^{(2)} \\ T^{(3)} \end{pmatrix} \ . \tag{VI.49}$$

We note the following identity: Let A and B be operators, then we find

$$
\begin{aligned}
\begin{pmatrix} 0 & A \\ B & 0 \end{pmatrix}^2 &= \begin{pmatrix} AB & 0 \\ 0 & BA \end{pmatrix} \\
\sum_{n=0}^{\infty} \begin{pmatrix} 0 & A \\ B & 0 \end{pmatrix}^n &= \sum_{l=0}^{\infty} \begin{pmatrix} 0 & A \\ B & 0 \end{pmatrix}^{2l} + \begin{pmatrix} 0 & A \\ B & 0 \end{pmatrix}^{2l+1} = \\
&= \sum_{l=0}^{\infty} \begin{pmatrix} AB & 0 \\ 0 & BA \end{pmatrix}^l + \begin{pmatrix} AB & 0 \\ 0 & BA \end{pmatrix}^l \begin{pmatrix} 0 & A \\ B & 0 \end{pmatrix} = \\
&= \sum_{l=0}^{\infty} \begin{pmatrix} AB & 0 \\ 0 & BA \end{pmatrix}^l \begin{pmatrix} \mathbb{1} & A \\ B & \mathbb{1} \end{pmatrix} = \\
&= \sum_{l=0}^{\infty} \begin{pmatrix} (AB)^l & 0 \\ 0 & (BA)^l \end{pmatrix} \begin{pmatrix} \mathbb{1} & A \\ B & \mathbb{1} \end{pmatrix} = \\
&= \begin{pmatrix} (1-AB)^{-1} & 0 \\ 0 & (1-BA)^{-1} \end{pmatrix} \begin{pmatrix} \mathbb{1} & A \\ B & \mathbb{1} \end{pmatrix} .
\end{aligned}
\tag{VI.50}
$$

We thus get

$$
\begin{pmatrix} T_2 \\ T_3 \end{pmatrix} = \begin{pmatrix} \left(1 - T^{(2)} G_0 T^{(3)} G_0\right)^{-1} & 0 \\ 0 & \left(1 - T^{(3)} G_0 T^{(2)} G_0\right)^{-1} \end{pmatrix} \begin{pmatrix} \mathbb{1} & T^{(2)} G_0 \\ T^{(3)} G_0 & \mathbb{1} \end{pmatrix} \begin{pmatrix} T^{(2)} \\ T^{(3)} \end{pmatrix} . \tag{VI.51}
$$

This equation yields the full T-operator by simply multiplying with the row-vector $(\mathbb{1}\ \mathbb{1})$ and thus contains all the singularities of the full T-operator. We distinguish the case where either $V^{(2)}$ or $V^{(3)}$ identically vanish and the case where both are not equal to 0. In the first case with $V^{(3)} = 0$ ($V^{(2)} = 0$ is completely analogous) we find

$$
T_2 = T^{(2)} = \left(1 - V^{(2)} G_0\right)^{-1} V^{(2)} \tag{VI.52}
$$

thus we have a singularity, if

$$
\mathbf{det}\left(1 - V^{(2)} G_0\right) = 0 \tag{VI.53}
$$

which was our result for the two-particle case. In the more general case with $V^{(2)} \neq 0$ and $V^{(3)} \neq 0$ we find two conditions and the T-operator is singular if either of these two conditions is satisfied

$$\begin{aligned} \mathbf{det}\left(1 - T^{(2)}G_0T^{(3)}G_0\right) &= 0 \\ \mathbf{det}\left(1 - T^{(3)}G_0T^{(2)}G_0\right) &= 0 \ . \end{aligned} \tag{VI.54}$$

Similar to the two-particle case these equations can be limited to a restricted Hilbert-space given by the projection operators $P^{(2)}$ and $P^{(3)}$ which satisfy

$$\begin{aligned} V^{(2)} &= P^{(2)}V^{(2)} = P^{(2)}V^{(2)} \\ V^{(3)} &= P^{(3)}V^{(3)} = P^{(3)}V^{(3)} \ . \end{aligned} \tag{VI.55}$$

This yields

$$\begin{aligned} \mathbf{det}\left(1 - T^{(2)}G_0T^{(3)}G_0P^{(2)}\right) &= 0 \\ \mathbf{det}\left(1 - T^{(3)}G_0T^{(2)}G_0P^{(3)}\right) &= 0 \end{aligned} \tag{VI.56}$$

for the case $V^{(2)} \neq 0$ and $V^{(3)} \neq 0$. Notice that these two determinants are identical by the Weinstein-Aronszajn identity, thus we can restrict our attention to the second equation

$$\mathbf{det}\left(1 - T^{(3)}G_0T^{(2)}G_0P^{(3)}\right) = 0 \ . \tag{VI.57}$$

Here, we notice the problem with three particles in the fact that $P^{(3)}$ maps to a finite dimensional Hilbert-space, if the genuine three-particle interactions only have a finite range, while $P^{(2)}$ always maps to an infinite dimensional space in the three-particle sector. Therefore we reduced the determinant again to a determinant of a finite matrix but now we are faced with the challenge to calculate the operator $T^{(2)}$ which includes the inversion of an operator on the infinite dimensional subspace given by $P^{(2)}$.
We can rewrite this equation in a similar way to the two-particle case using the exclusive two-particle Green's function

$$G^{(2)}(z) = \left(z - H_0 - V^{(2)}\right)^{-1} \tag{VI.58}$$

as

$$\mathbf{det}\left(1 - T^{(3)}\left(G^{(2)} - G_0\right)P^{(3)}\right) = 0 \ . \tag{VI.59}$$

Here we shifted the challenge to the calculation of $G^{(2)}(z)$ which again involves the inversion of an operator on an infinite dimensional subspace.
A special case that still allows the effective use of this method in the three-particle sector are bosonic or fermionic models without two-particle interactions that only contain genuine short-range three-particle interactions as for them the entire interaction again only has a finite dimensional image even in the three-particle sector. A toy model specifically constructed to satisfy these criteria is studied in Appendix C. Any application to real physical models of interest seems severely limited due to the strong requirement of the absence of two-particle interactions.
An attempt to approximate the correct equations can be made by replacing all two-particle interactions with long-range three-particle interactions via the insertion of a particle counting operator $N = \sum_i n_i$

$$b_{i_1}^\dagger b_{i_2}^\dagger b_{i_3} b_{i_4} \to \sum_i b_{i_1}^\dagger b_{i_2}^\dagger n_i b_{i_3} b_{i_4} = \sum_i b_{i_1}^\dagger b_{i_2}^\dagger b_i^\dagger b_i b_{i_3} b_{i_4} \ . \tag{VI.60}$$

these interactions can than be cut-off when the three particles are to far apart. This method has the advantage that the hopping is still treated correctly in the thermodynamic limit and the continuum consisting out of three quasi-free particles is correctly described. The disadvantage lies in the 2+1 continuum that consists out of one quasi-free particle and one quasi-free two-particle bound-state. This continuum will not be present as a continuum but instead will look like a large amount of three-particle bound-states close together. In the limit where the cut-off vanishes these states will form the 2+1 continuum. Identifying a true three-particle bound-state using this cut-off approximation can therefore be challenging, as it is not trivial to determine a true three particle bound-state among these state converging towards the 2+1 continuum.
Another approach lies in obtaining series expansions for the matrix elements of the exclusive two-particle Green's function $G^{(2)}(z)$, as usually only finitely many matrix equations are required to evaluate equation (VI.59). Here standard perturbative techniques for the evaluation of matrix elements of inverse operators can be used. But difficulties arise if an non-trivial interaction is present in the first non-trivial order of the operator $H_0 + V^{(2)}$.

VI.1.6 Mapping a hard-core boson problem to a boson model

To apply the previously discussed ansatz to a system described by hard-core bosonic excitations like spin-1/2 models, we need to map the hard-core bosonic creation and annihilation operators to bosonic ones. This transformation should also exclude any infinite repulsive onsite interactions, as they introduce a significant challenge in their analytic treatment. A similar ansatz was employed in reference [23] to calculate the

series expansion for the two-triplon (anti-)bound-states on the Heisenberg ladder. Consider a Hamiltonian that is the sum of products of hard-core bosonic creation and annihilation operators $a^\dagger_{\alpha,i}$, $a_{\alpha,i}$. We can introduce corresponding bosonic creation and annihilation operators $b^\dagger_{\alpha,i}$, $b_{\alpha,i}$ at each site i and of flavour α. Simply replacing $a^\dagger_{\alpha,i} \to b^\dagger_{\alpha,i}$ will change the fundamental problem as now multiple particle can reside at one site. Alongside the bosonic operators a bosonic Hilbert space $\mathbb{H}^{\mathbb{B}}$ is introduced that admits multiple particles at a given site. We denote the subspace of $\mathbb{H}^{\mathbb{B}}$ that admits at most m particles at any site by $\mathbb{H}^{\mathbb{B}}_m$. The operators $b^\dagger_{\alpha,i}$ do not conserve these subspaces, while the operators $b_{\alpha,i}$ do. This is why the simple substitution $a^\dagger_{\alpha,i} \to b^\dagger_{\alpha,i}$ with a restriction to $\mathbb{H}^{\mathbb{B}}_{m=1}$ fails. Instead we introduce the substitution

$$a^\dagger_{\alpha,i} \to b^\dagger_{\alpha,i} P^0_i \tag{VI.61}$$

where P^0_i is the projection operator on the subspace with 0 particles at site i. It is easy to show that

- $b^\dagger_{\alpha,i} P^0_i$ conserves the subspace $\mathbb{H}^{\mathbb{B}}_1$.
- On $\mathbb{H}^{\mathbb{B}}_1$ $b^\dagger_{\alpha,i} P^0_i$ acts like a hard-core bosonic creation operator.

If we further assume that the total number of hard-core bosons is fixed to some finite number N in the initial Hamiltonian, we can write the projection operator as

$$\begin{aligned} P^0_i &= \prod_\alpha \prod_{l=1}^{N} \left(1 - \frac{n_{\alpha,i}}{l}\right) \ , \\ n_{\alpha,i} &= b^\dagger_{\alpha,i} b_{\alpha,i} \ . \end{aligned} \tag{VI.62}$$

To conserve the Hermitian nature of the initial Hamiltonian we will also introduce the replacement

$$a_{\alpha,i} \to P^0_i b_{\alpha,i} \ . \tag{VI.63}$$

Note that on the subspace $\mathbb{H}^{\mathbb{B}}_1$ the replacement $a_{\alpha,i} \to b_{\alpha,i}$ would already be sufficient. The new Hamiltonian defined by the above substitutions is therefore equivalent to the hard-core bosonic Hamiltonian on the subspace $\mathbb{H}^{\mathbb{B}}_1$ and also conserves this subspace. The original hard-core bosonic problem can now be studied on the full bosonic subspace $\mathbb{H}^{\mathbb{B}}$ using the new bosonic Hamiltonian, which is known to be block diagonal with respect to the subspace $\mathbb{H}^{\mathbb{B}}_1$. Solving for the relevant eigenstates and their energies of the hard-core bosonic thus is equivalent to determining the eigenstates and energies of

the bosonic problem and checking if the solutions found lie in the subspace $\mathbb{H}_1^{\mathbb{B}}$. Note that the hard-core bosonic nature of the original particle gets absorbed in additional interaction terms on the bosonic subspace $\mathbb{H}^{\mathbb{B}}$, the simplest example of which will be discussed in the following section.

VI.1.6.1 Example: Two free hard-core bosons

We want to study the Hamiltonian of two free hard-core bosons on a chain described by nearest-neighbour hopping

$$H = J \sum_i a_{i+1}^\dagger a_i + a_i^\dagger a_{i+1} \tag{VI.64}$$

We can now introduce the substitution to bosons to obtain the bosonic Hamiltonian

$$H^{\mathbb{B}} = J \sum_i b_{i+1}^\dagger P_{i+1}^0 P_i^0 b_i + b_i^\dagger P_i^0 P_{i+1}^0 b_{i+1} \ . \tag{VI.65}$$

We will restrict this Hamiltonian to the subspace with at most one boson at each site and a total number of two bosons denoted by $\mathbb{H}_1^{\mathbb{B}}|_2 = \mathbb{H}_1^{\mathbb{B}} \cap \mathbb{H}|_2$. On this subspace we find

$$\begin{aligned} P_i^0 &= \left(1 - n_i\right)\left(1 - \frac{n_i}{2}\right) \\ &= 1 - \frac{3}{2} n_i + \frac{n_i^2}{2} \\ &= 1 - n_i \ . \end{aligned} \tag{VI.66}$$

Thus the bosonic Hamiltonian becomes

$$\begin{aligned} H^{\mathbb{B}} &= J \sum_i b_{i+1}^\dagger P_{i+1}^0 P_i^0 b_i + b_i^\dagger P_i^0 P_{i+1}^0 b_{i+1} \\ &= J \sum_i b_{i+1}^\dagger b_i - b_{i+1}^\dagger (n_{i+1} + n_i) b_i + b_{i+1}^\dagger n_{i+1} n_i b_i + \text{h.c.} \\ &= J \sum_i b_{i+1}^\dagger b_i - b_{i+1}^\dagger b_{i+1}^\dagger b_{i+1} b_i - b_{i+1}^\dagger b_i^\dagger b_i b_i + b_{i+1}^\dagger b_{i+1}^\dagger b_i^\dagger b_{i+1} b_i b_i + \text{h.c.} \\ &= J \sum_i b_{i+1}^\dagger b_i - b_{i+1}^\dagger b_{i+1}^\dagger b_{i+1} b_i - b_{i+1}^\dagger b_i^\dagger b_i b_i + \text{h.c.} \end{aligned} \tag{VI.67}$$

where we could drop the last term, as we are restricted to the two particle subspace. Note how each term individually fails to conserve the $\mathbb{H}_1^{\mathbb{B}}$ subspace but the sum of all terms manages to conserve it. For most applications it will be the easiest method to solve this Hamiltonian in the full two-particle subspace $\mathbb{H}|_2$ and afterwards selecting only those solutions also in the $\mathbb{H}_1^{\mathbb{B}}$ subspace. This also demonstrates why even free hard-core bosons pose significant challenges as they map to a system of interacting bosons.

VI.1.7 Examples

We will show three examples for this method. In the first example we will reproduce the analytical result for the two-particle bound-state energy of the one-dimensional XXZ-model (see section IV.1.1). After that we will apply the method to the two-dimensional XXZ model to demonstrate how we can study models which are not one-dimensional and that do not posses analytical solutions. In the end we will use the Green's function method in order to obtain a perturbative bound-state series expansion of the two-triplon bound-states of the Heisenberg ladder with additional cross terms (see section IV.2.3).

VI.1.7.1 Two-particle bound-state energy of the XXZ-model

We first want to test the Green's function method to obtain the analytical results for the one-dimensional two-particle bound-states of the XXZ-model (see section IV.1.1)

$$H = \frac{J}{2}\sum_i a_{i+1}^\dagger a_i + a_i^\dagger a_{i+1} - \lambda \sum_i n_{i+1} n_i \ . \tag{VI.68}$$

In this model only one particle flavour is present and the maximum range of the hopping and interaction is given by one site. Since this is a hard-core boson problem, we have to perform the boson mapping VI.1.6 first. The subspace the interaction operator acts on non-trivially is thus two-dimensional spanned by the two vectors $|K,0\rangle$ and $|K,1\rangle$ in the (K,d)-basis (see equation (VI.21)). The interaction in the boson Hilbert space is given by

$$\begin{aligned} V &= V^{\mathbb{B}} + V^C \\ V^{\mathbb{B}} &= \begin{pmatrix} 0 & 0 \\ 0 & -\lambda \end{pmatrix} \\ V^C &= -\sqrt{2}J \begin{pmatrix} 0 & \cos(K/2)e^{-iK/2} \\ \cos(K/2)e^{iK/2} & 0 \end{pmatrix} , \end{aligned} \tag{VI.69}$$

with the initial interaction $V^{\mathbb{B}}$ in the bosonic Hilbert space $\mathbb{H}|_2$ and the correction due to the hard-core boson to boson mapping V^C, as discussed in the previous section VI.1.6. The two-particle dispersion is given by

$$\omega(k_1, k_2) = J\left(\cos(k_1) + \cos(k_2)\right) \ . \tag{VI.70}$$

The free Green's function corresponds to

$$G_0(z) = \frac{1}{z - H_0} = \sum_{\boldsymbol{k}_1, \boldsymbol{k}_2} \frac{1 + \delta_{\boldsymbol{k}_1, \boldsymbol{k}_2}}{2} \frac{|\boldsymbol{k}_1, \boldsymbol{k}_2\rangle \langle \boldsymbol{k}_1, \boldsymbol{k}_2|}{z - \omega(\boldsymbol{k}_1, \boldsymbol{k}_2)} \ . \tag{VI.71}$$

Following equation (VI.24) we find the matrix elements of the free Green's function in the (K,d)-basis

$$G_0(z) = \begin{pmatrix} \frac{1}{2} I_{0,0}(K, z) & \frac{1}{\sqrt{2}} e^{-iK/2} I_{0,1}(K, z) \\ \frac{1}{\sqrt{2}} e^{iK/2} I_{1,0}(K, z) & I_{1,1}(K, z) \end{pmatrix} \ . \tag{VI.72}$$

The Brillouin zone integrals in the one particle flavour case are in general given by equation (VI.26) and here specifically by

$$I_{d,d'}(K, z) = \frac{1}{\pi} \int_0^{2\pi} \frac{\cos\left(d(k - K/2)\right) \cos\left(d'(k - K/2)\right)}{z - J\left(\cos(k) + \cos(K - k)\right)} dk \ . \tag{VI.73}$$

In order to calculate the implicit equation (VI.13) we first calculate the matrix $\mathbb{1} - PG_0(z)V$, which for this problem takes the form

$$\begin{aligned} &\mathbb{1} - PG_0(V^{\mathrm{C}} + V^{\mathbb{B}}) = \\ &= \begin{pmatrix} 1 + J\cos(K/2) I_{0,1} & \frac{1}{\sqrt{2}} J\cos(K/2) e^{-iK/2} I_{0,0} + \frac{1}{\sqrt{2}} \lambda e^{-iK/2} I_{0,1} \\ \sqrt{2} J\cos(K/2) I_{1,1} e^{iK/2} & 1 + J\cos(K/2) I_{1,0} + \lambda I_{1,1} \end{pmatrix} \ . \end{aligned} \tag{VI.74}$$

The determinant of this matrix is equivalent to the implicit function (VI.33) given by

$$\begin{aligned} f(z, K) &= \mathbf{det}\left(\mathbb{1} - PG_0(z, K)(V^{\mathrm{C}}(K) + V^{\mathbb{B}})\right) = \\ &= J^2 \cos^2(K/2)(I_{0,1}^2 - I_{0,0} I_{1,1}) + (2J\cos(K/2) I_{0,1} + \lambda I_{1,1}) + 1 \ . \end{aligned} \tag{VI.75}$$

The value of the bound-state energy ϵ is equivalent to the root of the implicit function $f(z, K)$ in z. We will investigate the two points $K = 0$ and $K = \pi$ to illustrate the solution to this implicit equation. For these values the integrals are given by

$$
\begin{aligned}
I_{0,0}(\pi, z) &= \frac{1}{\pi}\int_0^{2\pi} \frac{1}{z - J\left(\cos(k) + \cos(k-\pi)\right)} dk = \frac{2}{z} \\
I_{0,1}(\pi, z) &= \frac{1}{\pi}\int_0^{2\pi} \frac{\cos\left(k - \pi/2\right)}{z - J\left(\cos(k) + \cos(k-\pi)\right)} dk = 0 \\
I_{1,1}(\pi, z) &= \frac{1}{\pi}\int_0^{2\pi} \frac{\cos^2\left(k - \pi/2\right)}{z - J\left(\cos(k) + \cos(k-\pi)\right)} dk = \frac{1}{z}
\end{aligned}
\tag{VI.76}
$$

$$
\begin{aligned}
I_{0,0}(0, z) &= \frac{1}{2\pi}\int_0^{\pi} \frac{1}{z - 2J\cos(k)} dk = 2\frac{\mathrm{sign}(z)}{\sqrt{z^2 - 4J^2}} \\
I_{0,1}(0, z) &= \frac{1}{\pi}\int_0^{2\pi} \frac{\cos\left(k\right)}{z - 2J\cos(k)} dk = \frac{1}{J}\left(\frac{|z|}{\sqrt{z^2 - 4J^2}} - 1\right) \\
I_{1,1}(0, z) &= \frac{1}{\pi}\int_0^{2\pi} \frac{\cos^2\left(k\right)}{z - 2J\cos(k)} dk = \frac{z}{2J^2}\left(\frac{|z|}{\sqrt{z^2 - 4J^2}} - 1\right)
\end{aligned}
$$

with $|z/J| > 2$ in the case $K = 0$. Inserting these results into the implicit function (VI.75) and equating to zero yields

$$
f(z, K = \pi) = \frac{\lambda}{z} + 1 = 0 \tag{VI.77}
$$

for $K = \pi$, resulting in $z = -\lambda$. While for $K = 0$ we obtain

$$
f(z, K = 0) = \left(\frac{|z|}{\sqrt{z^2 - 4J^2}} - 1\right)\left(1 + \frac{\lambda z}{2J^2}\right) + 1 = 0 \ , \tag{VI.78}
$$

where we can readily check that $z = -\left(\lambda + \frac{J^2}{\lambda}\right)$ is a solution for all $\lambda/J > 1$. We again recover the established results for the bound-state energy from section IV.1.1. The property that a bound-state at $K = 0$ only exists for $\lambda/J > 1$ becomes apparent looking at the implicit function $f(z, K)$ of this problem in figure VI.1. This figure depicts the implicit function as a function of z for the total momentum values of $K = 0$ and $K = \pi$. We notice that at $K = \pi$ a bound-state, i.e. a root of $f(z, K)$ in z, always exists, while for $K = 0$ only a sufficiently large $\lambda/J > 1$ yields a root of the function below the energy of the two-particle continuum denoted by the red line. The general behaviour of the implicit function can be inferred from its definition via equation (VI.13). We now that in the limit of large $|z|$ the implicit function converges towards 1 and we usually observe that the implicit function diverges at the edges of the two-particle continuum due to the divergence of the free Green's function (VI.20). Assuming these two properties hold, we can conclude that at least one bound-state has

to exist, if the implicit function diverges to negative infinity at the lower edge of the two-particle continuum (red line in figure VI.1). This behaviour can be observed in the figure below, as well as the special case $\lambda/J = 1$ at $K = 0$ where the implicit function changes its behaviour at the lower edge of the two-particle continuum from divergence to positive ($\lambda/J < 1$) to negative ($\lambda/J > 1$) infinity. At the point $\lambda/J = 1$ at $K = 0$ the limit of the implicit function at the lower edge of the two-particle continuum is finite and equal to 1.

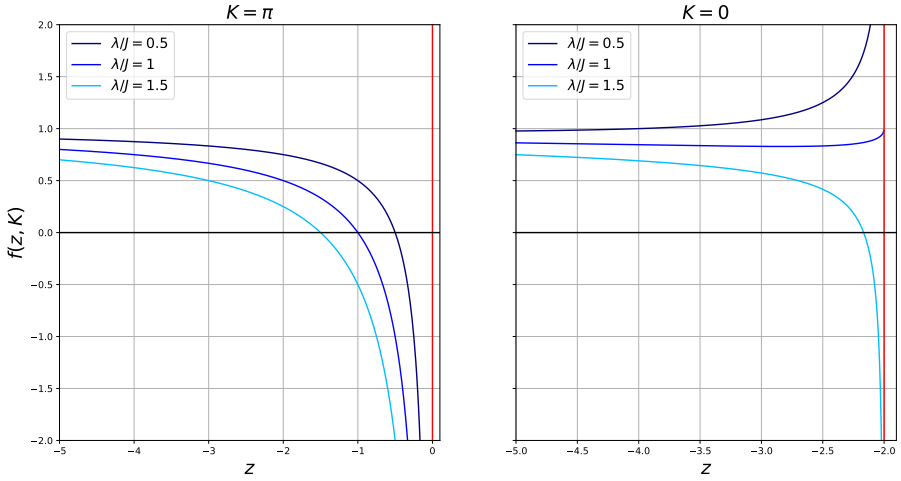

Figure VI.1: Implicit function $f(z, K)$ of the one dimensional XXZ model for total momentum $K = \pi$ left and $K = 0$ right and a range of interaction strengths λ/J. Any root of the implicit function corresponds to a two-particle bound-state. The energy of the lower edge of the two-particle continuum is shown via the red line.

VI.1.7.2 Two-particle bound-state energy of the two dimensional XXZ model

Next, we investigate the two dimensional XXZ model with nearest neighbour interaction on a square lattice

$$H = \frac{1}{2} \sum_{<i,j>} a_i^\dagger a_j + \text{h.c.} - \lambda \sum_{<i,j>} n_i n_j \ . \tag{VI.79}$$

After the boson mapping the Hamiltonian reads

$$H = \frac{1}{2} \sum_{<i,j>} b_i^\dagger b_j + \text{h.c.} - \lambda \sum_{<i,j>} n_i n_j - \frac{1}{2} \sum_{<i,j>} b_i^\dagger (n_i + n_j) b_j + \text{h.c.} \ . \tag{VI.80}$$

We take the hopping part as our free Hamiltonian. Analogous to the one dimensional case we define the Fourier transform and eigenstates of the free Hamiltonian

$$\begin{aligned} b_{\boldsymbol{k}}^\dagger &= \frac{1}{N}\sum_{\boldsymbol{r}} e^{i\boldsymbol{r}\boldsymbol{k}} b_{\boldsymbol{r}}^\dagger \\ b_{\boldsymbol{k}} &= \frac{1}{N}\sum_{\boldsymbol{r}} e^{-i\boldsymbol{r}\boldsymbol{k}} b_{\boldsymbol{r}} \end{aligned} \tag{VI.81}$$

and

$$|\boldsymbol{k}_1, \boldsymbol{k}_2\rangle = \sqrt{\frac{2-\delta_{\boldsymbol{k}_1,\boldsymbol{k}_2}}{2}} b_{\boldsymbol{k}_1}^\dagger b_{\boldsymbol{k}_2}^\dagger |0\rangle \ . \tag{VI.82}$$

We find a small difference in the definition of the two dimensional analogue to the (K,d)-basis

$$|\boldsymbol{K}, \boldsymbol{d}\rangle = \sqrt{\frac{2-\delta_{\boldsymbol{d},\boldsymbol{0}}}{2}} \frac{1}{\sqrt{N}} \sum_{\boldsymbol{r}} e^{i\boldsymbol{r}\boldsymbol{K}} b_{\boldsymbol{r}}^\dagger b_{\boldsymbol{r}+\boldsymbol{d}}^\dagger |0\rangle \tag{VI.83}$$

namely that the vector $\boldsymbol{d}$ is now restricted to a half plane say, $d_x \geq 0$, as the case with negative d_x is identical to the case where we flip $\boldsymbol{d} \to -\boldsymbol{d}$ due to the indistinguishability of the two particles. This also gives the restriction $d_y \geq 0$ if $d_x = 0$.
Since both the interaction as well as the hopping are only NN, we have to consider the three values of

$$\boldsymbol{d} \in \{(0,0), (1,0), (0,1)\} \ . \tag{VI.84}$$

The free Green's function is given by

$$\begin{aligned} G_0(z) = \frac{1}{z - H_0} &= \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2} \frac{1+\delta_{\boldsymbol{k}_1,\boldsymbol{k}_2}}{2} \frac{|\boldsymbol{k}_1,\boldsymbol{k}_2\rangle \langle \boldsymbol{k}_1,\boldsymbol{k}_2|}{z - \omega(\boldsymbol{k}_1,\boldsymbol{k}_2)} \\ \omega(\boldsymbol{k}_1,\boldsymbol{k}_2) &= \cos(k_{1,x}) + \cos(k_{1,y}) + \cos(k_{2,x}) + \cos(k_{2,y}) \ . \end{aligned} \tag{VI.85}$$

The remaining calculations are identical to the one dimensional cases by simply replacing d and k by their vector equivalences. In the (K,d)-basis the relevant matrices are given by

$$
\begin{aligned}
V^{\mathbb{B}} &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & -\lambda & 0 \\ 0 & 0 & -\lambda \end{pmatrix} \\
V^{C} &= -\sqrt{2} \begin{pmatrix} 0 & \cos(K_x/2)e^{-iK_x/2} & \cos(K_y/2)e^{-iK_y/2} \\ \cos(K_x/2)e^{iK_x/2} & 0 & 0 \\ \cos(K_y/2)e^{iK_y/2} & 0 & 0 \end{pmatrix} \\
G_0(z) &= \begin{pmatrix} \frac{1}{2} I_{\mathbf{0},\mathbf{0}} & \frac{1}{\sqrt{2}} e^{-iK_x/2} I_{(1,0),\mathbf{0}} & \frac{1}{\sqrt{2}} e^{-iK_y/2} I_{(0,1),\mathbf{0}} \\ \frac{1}{\sqrt{2}} e^{iK_x/2} I_{(1,0),\mathbf{0}} & I_{(1,0),(1,0)} & e^{i(K_x-K_y)/2} I_{(1,0),(0,1)} \\ \frac{1}{\sqrt{2}} e^{iK_y/2} I_{(0,1),\mathbf{0}} & e^{-i(K_x-K_y)/2} I_{(0,1),(1,0)} & I_{(0,1),(0,1)} \end{pmatrix}
\end{aligned}
\tag{VI.86}
$$

at a fixed total momentum $\boldsymbol{K}$ with the integrals

$$
I_{\boldsymbol{d},\boldsymbol{d'}}(\boldsymbol{K}, z) = \frac{2}{A_{\mathrm{BZ}}} \int_{1.\mathrm{BZ}} \frac{\cos\left(\boldsymbol{d}(\boldsymbol{k} - \boldsymbol{K}/2)\right) \cos\left(\boldsymbol{d'}(\boldsymbol{k} - \boldsymbol{K}/2)\right)}{z - \omega(\boldsymbol{k}, \boldsymbol{K} - \boldsymbol{k})} d\boldsymbol{k} \ . \tag{VI.87}
$$

The implicit equation for the eigenenergies is then given by

$$
\mathbf{det}\left(1 - PG_0(z)\left(V^C + V^{\mathbb{B}}\right)\right) = 0 \ . \tag{VI.88}
$$

We can now study this implicit equation at fixed values of the total momentum $\boldsymbol{K}$ and λ as a function of z

$$
f(z, \boldsymbol{K}) = \mathbf{det}\ \left(1 - PG_0(z, \boldsymbol{K})\left(V^C + V^{\mathbb{B}}(\boldsymbol{K})\right)\right) \tag{VI.89}
$$

where the roots of $f(z, \boldsymbol{K})$ in z define the bound-state energies of the model. Figure VI.2 depicts this function as a function of z for the values $\boldsymbol{K} = (\pi, \pi)$ and $\boldsymbol{K} = (\pi, \pi/2)$ of the total momentum. We clearly see whether a bound-state is present by the roots of the function. As in the previous example the function diverges at the energy of the lower edge of the continuum (red line). In contrast to the previous one dimensional case we have up to two bound-states present. At a momentum of $K = (\pi, \pi)$ we see roots with multiplicity two corresponding to the two-fold degeneracy of the corresponding eigenenergies of the bound-states. At $K = (\pi/2, \pi)$ we notice the splitting of the degenerate eigenenergies into two distinct bound-states, while for sufficiently small values of the interaction λ only one bound-state is present.

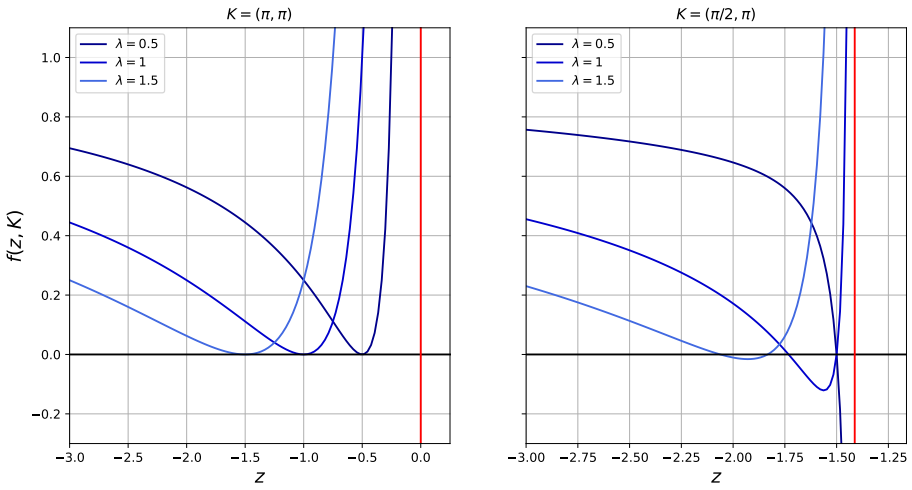

Figure VI.2: Implicit function $f(z, K)$ of the two dimensional XXZ model on a square lattice for total momentum $K = (\pi, \pi)$ left and $K = (\pi/2, \pi)$ right and a range of interaction strengths λ. The energy of the lower edge of the two-particle continuum is shown via the red line.

VI.1.7.3 Two-triplon bound-state series in the Heisenberg ladder with cross terms

We will use the Green's function method to obtain a series expansion for the two-triplon total spin-0 bound-state of the Heisenberg ladder with additional cross terms IV.2.3 out of the dimer limit. This is also an example for a unique problem arising in the series expansion of a bound-state energy in two variable. As discussed in V.1 to perform a series expansion around a bound-state we start not from the zeroth order Hamiltonian but from the first non-trivial order, which is the first order in this case. In first order in the total spin-zero sector the Hamiltonian (IV.22) (after rescaling by $1/J_\perp$) takes the from

$$H = h_0 \mathbb{1} + x_1 H^{(1)}_{x_1} + x_2 H^{(1)}_{x_2} + O(x_1^2, x_2^2, x_1 x_2) \ . \tag{VI.90}$$

We remove the zeroth order $h_0\mathbb{1}$ which is just a multiple of the identity in the two-triplon sector and use the first order as our undisturbed Hamiltonian. In one variable we would now be able to rescale the whole Hamiltonian by $1/x$ and start with $H^{(1)}$ as the undisturbed Hamiltonian but in two or more variables this is no longer possible as there are terms not proportional to perturbation parameter x_1. We solve this problem by introducing the ratio $r = x_2/x_1$ and rewrite the Hamiltonian as

$$H = x_1 H^{(1)}_{x_1} + x_1 r H^{(1)}_{x_2} + O(x_1^2) \ . \tag{VI.91}$$

Rescaling with $1/x_1$ we obtain

$$H = H^{(1)}_{x_1} + r H^{(1)}_{x_2} + O(x_1, r^2, x_1 r) \tag{VI.92}$$

where we now take $H^{(1)}_{x_1}$ as the undisturbed Hamiltonian and x_1 and r as perturbation parameters. This breaks the symmetry between x_1 and x_2 and one could also take $H^{(1)}_{x_2}$ as the undisturbed Hamiltonian by introducing the alternative ratio $\tilde{r} = x_1/x_2$. We can then explore the perturbation series of the bound states out of the three limits $r \ll 1$, $\tilde{r} \ll 1$ and $x_1 = x_2$ (the last limit can be calculated by performing perturbation theory in one variable). Here we will restrict our attention to the case $r \ll 1$ as this allows us to reproduce the series results by reference [23] and compare the coefficients to the ND based series expansion of this bound-state energy (see section V.1.1.1). The series expansions up to third-order at $K = \pi$ are given by

$$\begin{aligned}
\epsilon^{(2)}_{\text{Bound},S=0}(x_1, r, K = \pi) &= 2 - \frac{1}{1}x_1 + \frac{3}{4}x_1^2 - \frac{1}{1}rx_1 + \frac{5}{16}x_1^3 - \frac{3}{2}rx_1^2 \ , \\
\epsilon^{(2)}_{\text{Bound},S=1}(x_1, r, K = \pi) &= 2 - \frac{1}{2}x_1 + \frac{9}{8}x_1^2 - \frac{1}{2}rx_1 + \frac{5}{16}x_1^3 - \frac{9}{4}rx_1^2 \ ,
\end{aligned} \tag{VI.93}$$

where we considered the total spin-0 and total spin-1 subspace up to order $O(x_1^4, rx_1^3, r^2x_1^2, r^3x_1, r^4)$. The case $r = 0$ reproduces the results by reference [23] and matches the ND results V.1. The calculation of higher orders is possible for this system, but is eventually limited by the requirement to evaluate a large determinate with polynomial entries, as described in section VI.1.3. Calculating the determinant of a $n \times n$ matrix via its definition by Leibniz is of order $O(n!)$ and thus becomes quickly unfeasible. For matrix elements which possess an inverse (i.e. fields) fast algorithms of order $O(n^3)$ based on Gaussian elimination exist, but these are inaccessible to us due to the demand for inverses of the matrix entries. In this thesis we only calculated determinants using the slow $O(n!)$ algorithm, limiting our ability to calculate higher orders. In the future one should use faster algorithms for the evaluation of determinants over rings, which can be of order $O(n^4)$ (for details see reference [24]).

VI.2 Recursion relations for 1d systems

We want to give an overview how two-particle bound-states of one-dimensional hard-core boson models with short-range nearest-neighbour hopping and arbitrary density-density

interactions can be analytically studied. This technique is useful as such models are often derived as first-order effective Hamiltonians of one-dimensional models with long-range interactions and can be a starting-point for perturbative series expansions of two-particle bound-states using higher-order terms of the effective Hamiltonian. We will start by discussing this technique for systems with only one flavour of hard-core bosons and only nearest-neighbour hopping and later discuss ways to extend the results of this case to the more general case. A similar technique for systems with finite-range interactions was discussed in reference [25] and this ansatz was already used to solve models like the discrete Hydrogen atom on a one-dimensional chain [14].

VI.2.1 Systems with one hard-core boson flavour and nearest-neighbour hopping

This scenario is given by the long-range XXZ-model introduced in (IV.12)

$$H = -\frac{J}{2}\sum_i a_{i+1}^\dagger a_i + a_i^\dagger a_{i+1} - \sum_i \sum_{r=1}^{\infty} \lambda(r) n_{i+r} n_i \tag{VI.94}$$

The core idea of this method relies on the fact that we can reduce the Schrödinger-equation in one dimension to a simple recursion relation. We will again use the (K,d)-Basis to study this problem given by

$$|K;d\rangle = \sum_j e^{iK(j+d/2)} a_{j+d}^\dagger a_j^\dagger |0\rangle \ . \tag{VI.95}$$

We make the general ansatz for an eigenvector of fixed total momentum K

$$|\Psi\rangle = \sum_{d=1}^{\infty} g(d) |K;d\rangle \ . \tag{VI.96}$$

With this we can write the eigenvalue equation as

$$\begin{aligned} H|\Psi\rangle &= \epsilon|\Psi\rangle \\ \epsilon g(1) &= -J\cos(K/2)g(2) - \lambda(1)g(1) \\ \epsilon g(d) &= -J\cos(K/2)\left(g(d+1)+g(d-1)\right) - \lambda(d)g(d) \end{aligned} \tag{VI.97}$$

for $d > 1$. Without loss of generality we will choose $g(1) = 1$ thus giving

$$g(2) = g(2,\epsilon) = -\frac{\epsilon + \lambda(1)}{J\cos(K/2)} \ . \tag{VI.98}$$

Now, the second coefficient is known as a function of the eigenvalue ϵ. With $g(1)$ and $g(2)$ known we can use the second equation

$$g(d+1) = -\frac{\epsilon + \lambda(d)}{J\cos(K/2)} g(d) - g(d-1) \tag{VI.99}$$

to recursively define all the following coefficients as functions of the yet unknown eigenvalue ϵ. We now have defined functions $g(d, \epsilon)$ via the upper recursion relation (VI.99), which yield "eigenvectors"

$$|\Psi(\epsilon)\rangle = \sum_{d=1}^{\infty} g(d, \epsilon) \, |K; d\rangle \tag{VI.100}$$

for every number $\epsilon \in \mathbb{C}$. Usually not all numbers are eigenvalues of a given Hamiltonian. To determine the allowed eigenvalues we have to make sure that the resulting eigenvectors are normalisable. For a bound-state this results in the condition

$$\sum_{d=1}^{\infty} |g(d, \epsilon)|^2 < \infty \tag{VI.101}$$

while for quasi-free states the weaker condition

$$\lim_{d\to\infty} \left| \frac{g(d+1, \epsilon)}{g(d, \epsilon)} \right| = 1 \tag{VI.102}$$

is sufficient. This also leads to the necessary condition

$$\lim_{d\to\infty} g(d, \epsilon) = 0 \tag{VI.103}$$

for bound-states.
The analytical difficulty of this method is split into two steps. First the solution to the recursion equation (VI.99) has to be obtained. Generating functions are often a helpful tool to solve these kinds of equations, as they often transform the problem to a functional equation. The second difficult step is the determination of normalisable eigenstates. Here, it is often easier to first consider the necessary condition (VI.103) to find candidates for possible two-particle bound-state energies and afterwards the sufficient condition (VI.101) can be checked. In Appendix D the full calculations for the discrete one-dimensional Hydrogen atom $\lambda(d) = \frac{V}{d}$ and a model with exponentially decaying interactions $\lambda(d) = V\alpha^{d-1}$ are shown for $V > 0$, $\alpha < 1$. There we reproduce the results for the discrete one-dimensional Hydrogen atom (see reference [14]) and

show that for all attractive coupling strengths V an infinite amount of bound-states exists with an energy of

$$\epsilon_{\text{bound}}(m) = -\sqrt{\left(\frac{V}{m}\right)^2 + 4\cos^2(K/2)} \tag{VI.104}$$

for a total momentum of K and an integer quantum number m. For the exponentially decaying density-density interaction we find that in general only a finite amount of bound-states exists, with energies determined by the implicit equation

$${}_1\phi_1\left(0; \frac{\alpha}{x_2^2(\epsilon_{\text{bound}})}; \alpha, -\frac{V}{\cos(K/2)x_2(\epsilon_{\text{bound}})}\right) = 0\ . \tag{VI.105}$$

Here ${}_1\phi_1\left(\alpha;\beta;q,z\right)$ denotes a basic hypergeometric series. The bound-state energy ϵ_{bound} is included in the function

$$x_2(\epsilon) = \frac{1}{2\cos(K/2)}\left(\epsilon - \sqrt{\epsilon^2 - 4\cos^2(K/2)}\right)\ . \tag{VI.106}$$

In contrast to the discrete Hydrogen atom only finitely many bound-states exist for finite positive values of V and $\alpha < 1$.

VI.2.2 Longer-range hopping terms and multiple hard-core boson flavours

In the case that the hopping terms include next-nearest neighbour terms and more we have to modify the above ansatz. We will consider the case of an additional next-nearest neighbour hopping term

$$-\frac{J_2}{2}\sum_i a_{i+2}^\dagger a_i + a_i^\dagger a_{i+2} \tag{VI.107}$$

in the initial Hamiltonian (VI.94). While we are still free to choose $g(1) = 1$ the recursion relations now read

$$\begin{aligned}
H\left|\Psi\right\rangle &= \epsilon\left|\Psi\right\rangle \\
\epsilon g(1) &= -J\cos(K/2)g(2) - J_2\cos(K)g(1) - J_2\cos(K)g(3) - \lambda(1)g(1) \\
\epsilon g(2) &= -J\cos(K/2)\left(g(3)+g(1)\right) - J_2\cos(K)g(4) - \lambda(2)g(2) \\
\epsilon g(d) &= -J\cos(K/2)\left(g(d+1)+g(d-1)\right) - J_2\cos(K)\left(g(d+2)+g(d-2)\right) - \lambda(d)g(d)
\end{aligned} \tag{VI.108}$$

for $d > 2$. Thus if we would know $g(2)$ we could use the first equation to determine $g(3)$ and afterwards use the second equation to determine $g(4)$. When the first four values of $g(d)$ are known we can again use the last equation to recursively calculate

$$g(d+2) = -\frac{J\cos(K/2)}{J_2\cos(K)}\left(g(d+1)+g(d-1)\right) + \frac{\epsilon-\lambda(d)}{J_2\cos(K)}g(d) - g(d-2)\ . \quad \text{(VI.109)}$$

We therefore have to treat $g(2) \in \mathbb{C}$ as another free variable together with the unknown energy ϵ and calculate all coefficients as function of these two variables $g(d) \to g(d, \epsilon, g(2))$. Afterwards we proceed as before where we have to determine the eigenenergies ϵ and second coefficients $g(2)$ of bound-states via the normalisability criteria (VI.103), (VI.101). A generalisation to nth-nearest neighbour hopping is straightforward where now the coefficients $g(2), ..., g(n)$ have to be considered as free variables together with the eigenvalue ϵ.
We can use a similar strategy when dealing with multiple hard-core boson flavours. We consider the Hamiltonian

$$H = -\frac{1}{2}\sum_{\alpha,\beta}\sum_{i} J_{\alpha,\beta}a^\dagger_{i+1,\alpha}a_{i,\beta} + J^*_{\alpha,\beta}a^\dagger_{i,\beta}a_{i+1,\alpha} - \sum_{\alpha,\beta}\sum_{i}\sum_{r=1}^{\infty}\lambda_{\alpha,\beta}(r)n^\alpha_{i+r}n^\beta_i \quad \text{(VI.110)}$$

with $n^\alpha_i = a^\dagger_{i,\alpha}a_{i,\alpha}$. We introduce the (K,d)-Basis

$$|K;d;\alpha,\beta\rangle = \sum_j e^{iK(j+d/2)}a^\dagger_{j+d,\alpha}a^\dagger_{j,\beta}|0\rangle \quad \text{(VI.111)}$$

and the eigenstate ansatz for a total momentum K

$$|\Psi\rangle = \sum_{d=1}^{\infty} g(d,\alpha,\beta)\,|K;d;\alpha,\beta\rangle\ . \quad \text{(VI.112)}$$

Assuming a number of N_f different hard-core boson flavours we find that there are N_f^2 equations linking the N_f^2 coefficients $g(1,\alpha,\beta)$ for $\alpha,\beta \in \{1,...,N_f\}$ and the N_f^2 coefficients $g(2,\alpha,\beta)$ for $\alpha,\beta \in \{1,...,N_f\}$. Thus if all N_f^2 coefficients $g(1,\alpha,\beta)$ are known we can again recursively calculate the rest of the coefficients. We can only set one of these initial coefficients equal to 1 leaving us again with $N_f^2 - 1$ free variables that have to be considered in the normalisability conditions (VI.103), (VI.101).
A generalisation to multiple hard-core boson flavours and additional hopping terms is simply given by combining both methods leading to more free variables in the general "eigenvector".

In theory one can extent this ansatz to two or more dimensions by introducing more of these additional parameters but unlike in the one dimensional case even the case of one hard-core boson flavour with only nearest-neighbour hopping requires an infinite set of free parameters that have to be considered when determining the bound-state energy via the normalisation criterion (VI.101), thus making this ansatz not feasible in most higher dimensional models.

VII Summary and outlook

With the methods discussed in chapters V and VI we can study a wide range of bound-state systems. We are capable to reduce the problem of finding most two-particle bound-state energy to a finite implicit equation that operates fully in the thermodynamic limit using the Green's function method VI.1, removing the need for numerical diagonalisation and system size scaling in the two-particle sector. This method also allows us to calculate series expansions for the bound-state energy of two-particle bound-states directly in the thermodynamic limit. Regarding the three- and higher-particle sectors we can use perturbation theory and ND on finite systems V.1 to obtain series expansions for bound-states which exist in first non-trivial order and can effectively detect these bound-states using the scaling of the expectation value of the sum of particle distances in the system size using ND V.2. For two-particle bound-states which possess no series expansion around a perturbative limit, because they do not yet exist in first non-trivial order, the Green's function method allows us to obtain implicit functions of these energies that can be expanded and extrapolated in the perturbation parameter, which allows for the study of second order quantum phase transitions triggered by the closing of the two-particle bound-state energy gap VI.1.4. In studying the Green's function method we introduced a hard-core boson to boson mapping that does not utilise infinite onsite repulsion terms via the introduction of additional interactions on a larger Hilbert-space VI.1.6.
We also summarised the bound-state properties of the one-dimensional XXZ-model B and a technique to analytically study the two-particle bound-states on linear chains with potentially infinite range interaction VI.2 which are often useful for the study of low-order effective Hamiltonians.
Using these techniques we were able to reproduce and extend the results for the two-triplon bound-states of the Heisenberg ladder [2] VI.1.7 and show that in lowest order three triplon bound-states are present, which get more pronounced through higher order interactions [3]V.2.1.
Looking forward, the application of the Green's function method to the three- and higher-particle sector as discussed in VI.1.5 and the discovery and study of systems which display quantum phase transitions triggered by the closing of a two-particle bound-state gap have the potential for further study.

A Proving cluster additivity of general reduced matrix elements

We will prove that the irreducible m-particle matrix elements $\Delta^m_{i,j,k,\ldots;\alpha,\beta,\gamma,\ldots}$ are cluster additive via induction by consider two disconnected clusters A,B.
We start by proving the related property:
We define subsets of the indices $s_1 \subset \{i_1, ..., i_m\}$ and $s_2 \subset \{j_1, ..., j_m\}$ with $s_1, s_2 \in \mathrm{A}$ as well as their conjugated sets $\overline{s}_1$ and $\overline{s}_2$ with $\overline{s}_1, \overline{s}_2 \in \mathrm{B}$. We denote the irreducible matrix elements by

$$\Delta^m_{i_1,\ldots,i_m;j_1,\ldots,j_m} = \Delta^m_{s_1,\overline{s}_1;s_2,\overline{s}_2} \ . \tag{A.1}$$

We will prove via induction that $\Delta^m_{s_1,\overline{s}_1;s_2,\overline{s}_2}(\mathrm{A}) \neq 0$ only if $|s_1| = |s_2| = m$ for $m > 0$.
We start the induction by assuming the upper statement for all $0 < l < m$.
This statement is obvious if $|s_1| \neq |s_2|$, as we never have the same number of particles on the clusters A,B yielding zero for all expressions in equation (III.33).
If $0 < |s_1| = |s_2| = l < m$ we find the following expression

$$\sum_{n=1}^{m} A^n_{s_1,\overline{s}_1;s_2,\overline{s}_2}(\mathrm{A}) = \delta_{\overline{s}_1;\overline{s}_2} \sum_{n=0}^{l} A^n_{s_1;s_2}(\mathrm{A}) \tag{A.2}$$

where we used the initial assumption and $\langle s_1, \overline{s}_1 | s_2, \overline{s}_2 \rangle = \langle s_1 | s_2 \rangle \langle \overline{s}_1 | \overline{s}_2 \rangle = \delta_{s_1;s_2}\delta_{\overline{s}_1;\overline{s}_2}$.
Inserting this into the desired expression yields

$$\begin{aligned} \Delta^m_{s_1,\overline{s}_1;s_2,\overline{s}_2}(\mathrm{A}) &= h^l_{s_1;s_2}(\mathrm{A})\delta_{\overline{s}_1;\overline{s}_2} - \sum_{n=1}^{m} A^n_{s_1,\overline{s}_1;s_2,\overline{s}_2}(\mathrm{A}) \\ &= h^l_{s_1;s_2}(\mathrm{A})\delta_{\overline{s}_1;\overline{s}_2} - \delta_{\overline{s}_1;\overline{s}_2} \sum_{n=0}^{l} A^n_{s_1;s_2}(\mathrm{A}) \\ &= \left(h^l_{s_1;s_2}(\mathrm{A}) - h^l_{s_1;s_2}(\mathrm{A}) \right) \delta_{\overline{s}_1;\overline{s}_2} = 0 \end{aligned} \tag{A.3}$$

where we used the definition of the irreducible matrix element (III.33) in the last step.
The only remaining scenario is $|s_1| = |s_2| = 0$ which simply yields

$$\begin{aligned}\Delta^m_{s_1,\bar{s}_1;s_2,\bar{s}_2}(\mathrm{A}) &= h^0(\mathrm{A})\delta_{\bar{s}_1;\bar{s}_2} - \sum_{n=1}^{m} A^n_{s_1,\bar{s}_1;s_2,\bar{s}_2}(\mathrm{A}) \\ &= h^0(\mathrm{A})\delta_{\bar{s}_1;\bar{s}_2} - \delta_{\bar{s}_1;\bar{s}_2} h^0(A) = 0 \ .\end{aligned} \tag{A.4}$$

The induction is complete as we have already shown this property for $m = 1$ when discussing the irreducible one-particle matrix elements.
Next we will prove cluster additivity. First we assume cluster additivity for all irreducible matrix elements $\Delta^l_{s_1,\bar{s}_1;s_2,\bar{s}_2}$ with $l < m$, where we follow the previous notation. Starting with the trivial case $|s_1| \neq |s_2|$, where we need no induction to show cluster additivity as all irreducible matrix elements equal 0 in this case, due to the conservation of particle number. Considering the case $0 < |s_1| = |s_2| = l < m$ we find the following expression

$$\begin{aligned}&\sum_{n=1}^{m} A^n_{s_1,\bar{s}_1;s_2,\bar{s}_2}(\mathrm{A}\cup\mathrm{B}) = \sum_{k_1<k_2<\ldots<k_n}^{m} \sum_{l_1<l_2<\ldots<l_n}^{m} \delta_{i_{k_1},\ldots,i_{k_n};j_{l_1},\ldots,j_{l_n}} \\ &\times \left(\Delta^{m-n}_{i_1,\ldots,\widehat{i_{k_1}},\ldots,\widehat{i_{k_n}},\ldots,i_m;j_1,\ldots,\widehat{j_{l_1}},\ldots,\widehat{j_{k_n}},\ldots,j_m}(\mathrm{A}) + \right. \\ &\left. + \Delta^{m-n}_{i_1,\ldots,\widehat{i_{k_1}},\ldots,\widehat{i_{k_n}},\ldots,i_m;j_1,\ldots,\widehat{j_{l_1}},\ldots,\widehat{j_{k_n}},\ldots,j_m}(\mathrm{B}) \right) \\ &= \delta_{\bar{s}_1;\bar{s}_2} \sum_{n=0}^{l} A^n_{s_1;s_2}(\mathrm{A}) + \delta_{s_1;s_2} \sum_{n=0}^{m-l} A^n_{\bar{s}_1;\bar{s}_2}(\mathrm{B})\end{aligned} \tag{A.5}$$

where we used the assumed cluster additivity and the previous result (A.3). Inserting this into the desired expression yields

$$\begin{aligned}&\Delta^m_{s_1,\bar{s}_1;s_2,\bar{s}_2}(\mathrm{A}\cup\mathrm{B}) = h^l_{s_1;s_2}(\mathrm{A})\delta_{\bar{s}_1;\bar{s}_2} + \delta_{s_1;s_2} h^{m-l}_{\bar{s}_1;\bar{s}_2}(\mathrm{B}) - \sum_{n=1}^{m} A^n_{s_1,\bar{s}_1;s_2,\bar{s}_2}(\mathrm{A}\cup\mathrm{B}) \\ &= h^l_{s_1;s_2}(\mathrm{A})\delta_{\bar{s}_1;\bar{s}_2} + \delta_{s_1;s_2} h^{m-l}_{\bar{s}_1;\bar{s}_2}(\mathrm{B}) - \delta_{\bar{s}_1;\bar{s}_2} \sum_{n=0}^{l} A^n_{s_1;s_2}(\mathrm{A}) - \delta_{s_1;s_2} \sum_{n=0}^{m-l} A^n_{\bar{s}_1;\bar{s}_2}(\mathrm{B}) \\ &= \left(h^l_{s_1;s_2}(\mathrm{A}) - h^l_{s_1;s_2}(\mathrm{A}) \right) \delta_{\bar{s}_1;\bar{s}_2} + \delta_{s_1;s_2} \left(h^{m-l}_{\bar{s}_1;\bar{s}_2} - h^{m-l}_{\bar{s}_1;\bar{s}_2}(\mathrm{B}) \right) = 0 \\ &= \Delta^m_{s_1,\bar{s}_1;s_2,\bar{s}_2}(\mathrm{A}) + \Delta^m_{s_1,\bar{s}_1;s_2,\bar{s}_2}(\mathrm{B}) \ .\end{aligned} \tag{A.6}$$

We therefore showed not only cluster additivity but also the vanishing of the irreducible matrix element.

We are left with the case $|s_1| = |s_2| = m$ (which is identical to $|s_1| = |s_2| = 0$). We first consider the expression

$$\sum_{n=1}^{m} A^n_{s_1;s_2}(\mathrm{A} \cup \mathrm{B}) = \sum_{n=1}^{m} A^n_{s_1,\bar{s}_1;s_2,\bar{s}_2}(\mathrm{A}) + \delta_{s_1;s_2} h^0 \tag{A.7}$$

which yields

$$\begin{aligned} \Delta^m_{s_1;s_2}(\mathrm{A} \cup \mathrm{B}) &= h^m_{s_1;s_2}(\mathrm{A}) + \delta_{s_1;s_2} h^0 - \sum_{n=1}^{m} A^n_{s_1;s_2}(\mathrm{A} \cup \mathrm{B}) \\ &= h^m_{s_1;s_2}(\mathrm{A}) - \sum_{n=1}^{m} A^n_{s_1;s_2}(\mathrm{A}) = \Delta^m_{s_1;s_2}(\mathrm{A}) + 0 \\ &= \Delta^m_{s_1;s_2}(\mathrm{A}) + \Delta^m_{s_1;s_2}(\mathrm{B}) \end{aligned} \tag{A.8}$$

where we used equation (A.4) in the last step. We already showed that $\Delta^1_{s_1;s_2}$ is cluster additive thus finishing the prove by induction.

B Multi-particle bound states of the XXZ model in one dimension

We want to note that all these states are of the Bethe ansatz form, as the Hamiltonian

$$H = \sum_i a_{i+1}^\dagger a_i + \text{h.c.} - \lambda \sum_i n_{i+1} n_i \ . \tag{B.1}$$

is integrable using the Bethe ansatz. We want to restrict our attention to those states exponentially decaying in the distance between particles.
We start with $n+1$ particles on the chain. We will label those with the generalised (K,d)-basis defined as

$$\begin{aligned} &|K; d_1, ..., d_n\rangle = \\ &= \frac{1}{\sqrt{N}} \sum_j e^{\mathrm{i}K\left(j + \frac{1}{n+1}\sum_{l=1}^n (n+1-l)d_l\right)} |j, j+d_1, j+d_1+d_2, ..., j+d_1+...+d_n\rangle \ . \end{aligned} \tag{B.2}$$

We want to identify the action of the hopping-term on the general (K,d)-basis. To do this we look at what happens, if the m-th particle $(1 < m < n+1)$ hops one site to the right/left

$$\begin{aligned} &\frac{1}{\sqrt{N}} \sum_j e^{\mathrm{i}K\left(j + \frac{1}{n+1}\sum_{l=1}^n (n+1-l)d_l\right)} \\ &|j, j+d_1, ..., j+d_1+d_2+...+d_{m-1} \pm 1, ..., j+d_1+...+d_n\rangle = \\ &= \frac{1}{\sqrt{N}} \sum_j e^{\mathrm{i}K\left(j + \frac{1}{n+1}\sum_{l=1}^n (n+1-l)d_l\right)} e^{-\mathrm{i}K\left(\frac{\pm(n-m+2)}{n+1} + \frac{\mp(n-m+1)}{n+1}\right)} \\ &|j, ..., j+d_1+...+d_{m-1} \pm 1, j+d_1+...+(d_{m-1} \pm 1)+(d_m \mp 1), ...\rangle = \\ &e^{\mp \mathrm{i}\frac{K}{n+1}} |K; d_1, ..., d_{m-1} \pm 1, d_m \mp 1, ..., d_n\rangle \ . \end{aligned} \tag{B.3}$$

Here we just added ∓ 1 to the distance d_m and collected the correct phase factor to bring this expression into the (K,d)-Basis form.
For the left most particle we find

$$\begin{aligned}
&\frac{1}{\sqrt{N}}\sum_j e^{\mathrm{i}K\left(j+\frac{1}{n+1}\sum_{l=1}^{n}(n+1-l)d_l\right)}\,|j\pm 1, j+d_1, ..., j+d_1+...+d_n\rangle = \\
&= \frac{1}{\sqrt{N}}\sum_j e^{\mathrm{i}K\left(j+\frac{1}{n+1}\sum_{l=1}^{n}(n+1-l)d_l\right)} e^{-\mathrm{i}K\left(\pm 1+\frac{\mp n}{n+1}\right)} \\
&|j, j+(d_1\mp 1), ..., j+(d_1\mp 1)+...+d_n\rangle = \\
&e^{\mp\mathrm{i}\frac{K}{n+1}}\,|K; d_1\mp 1, ..., d_n\rangle
\end{aligned} \tag{B.4}$$

and analogously for the right most particle

$$\begin{aligned}
&\frac{1}{\sqrt{N}}\sum_j e^{\mathrm{i}K\left(j+\frac{1}{n+1}\sum_{l=1}^{n}(n+1-l)d_l\right)}\,|j, j+d_1, ..., j+d_1+...+d_n\pm 1\rangle = \\
&= \frac{1}{\sqrt{N}}\sum_j e^{\mathrm{i}K\left(j+\frac{1}{n+1}\sum_{l=1}^{n}(n+1-l)d_l\right)} e^{-\mathrm{i}K\left(\frac{\mp 1}{n+1}\right)} \\
&|j, j+d_1, ..., j+d_1+...+(d_n\pm 1)\rangle = \\
&e^{\mp\mathrm{i}\frac{K}{n+1}}\,|K; d_1, ..., d_n\pm 1\rangle \ .
\end{aligned} \tag{B.5}$$

With this we can write down the general ansatz for our bound-state

$$|\Phi\rangle = \sum_{d_1,...,d_n=1}^{\infty} A_1^{d_1}...A_n^{d_n}\,|K; d_1, ..., d_n\rangle \tag{B.6}$$

with n independent parameters $A_1, ..., A_n$. Acting with the Hamiltonian on this state yields

$$
\begin{aligned}
&H\,|\Phi\rangle = \\
=&e^{-\mathrm{i}\frac{K}{n+1}} \sum_{d_1,...,d_n=1}^{\infty} A_1^{d_1}...A_n^{d_n} \times \\
&\left(|K; d_1 - 1, ..., d_n\rangle + \sum_{m=1}^{n-1} |K; d_1, ..., d_m + 1, d_{m+1} - 1, ..., d_n\rangle + |K; d_1, ..., d_n + 1\rangle \right) + \\
+&e^{+\mathrm{i}\frac{K}{n+1}} \sum_{d_1,...,d_n=1}^{\infty} A_1^{d_1}...A_n^{d_n} \times \\
&\left(|K; d_1 + 1, ..., d_n\rangle + \sum_{m=1}^{n-1} |K; d_1, ..., d_m - 1, d_{m+1} + 1, ..., d_n\rangle + |K; d_1, ..., d_n - 1\rangle \right) - \\
-&\lambda \left(\sum_{m=1}^{n} \delta_{d_m,1} \right) |K; d_1, ..., d_n\rangle \ .
\end{aligned}
\tag{B.7}
$$

We can again use the identities obtained by shifting the summation

$$
\begin{aligned}
&\sum_{d_1,...,d_n=1}^{\infty} A_1^{d_1}...A_n^{d_n}\,|K; d_1, ..., d_m - 1, ..., d_n\rangle = \\
&= A_m \sum_{d_1,...,d_n=1}^{\infty} A_1^{d_1}...A_n^{d_n}\,|K; d_1, ..., d_m, ..., d_n\rangle \\
&\sum_{d_1,...,d_n=1}^{\infty} A_1^{d_1}...A_n^{d_n}\,|K; d_1, ..., d_m + 1, ..., d_n\rangle = \\
&= A_m^{-1} \sum_{d_1,...,d_n=1}^{\infty} A_1^{d_1}...A_n^{d_n}\,|K; d_1, ..., d_m, ..., d_n\rangle - \\
&- A_m^{-1} \sum_{d_1,...,d_{m-1},d_{m+1},d_n=1}^{\infty} A_1^{d_1}...A_n^{d_n}\,|K; d_1, ..., d_m = 1, ..., d_n\rangle
\end{aligned}
\tag{B.8}
$$

to obtain the result

$$
\begin{aligned}
& H\,|\Phi\rangle = \\
&= \left(e^{-\mathrm{i}\frac{K}{n+1}} \left(A_1 + \sum_{m=1}^{n-1} A_m^{-1} A_{m+1} + A_n^{-1} \right) + \right. \\
&\quad \left. + e^{+\mathrm{i}\frac{K}{n+1}} \left(A_1^{-1} + \sum_{m=1}^{n-1} A_m A_{m+1}^{-1} + A_n \right) \right) |\Phi\rangle - \\
&- \left(e^{\mathrm{i}\frac{K}{n+1}} A_1^{-1} + e^{-\mathrm{i}\frac{K}{n+1}} A_1^{-1} A_2 + \lambda \right) \sum_{d_2,\ldots,d_n=1}^{\infty} A_1^{d_1} \ldots A_n^{d_n} \,|K; d_1 = 1, \ldots, d_n\rangle - \\
&- \sum_{m=2}^{n-1} \left(e^{\mathrm{i}\frac{K}{n+1}} A_{m-1} A_m^{-1} + e^{-\mathrm{i}\frac{K}{n+1}} A_m^{-1} A_{m+1} + \lambda \right) \times \\
&\qquad \sum_{d_1,\ldots,d_{m-1},d_{m+1},\ldots,d_n=1}^{\infty} A_1^{d_1} \ldots A_n^{d_n} \,|K; d_1, \ldots, d_m = 1, \ldots, d_n\rangle - \\
&- \left(e^{\mathrm{i}\frac{K}{n+1}} A_{n-1} A_n^{-1} + e^{-\mathrm{i}\frac{K}{n+1}} A_n^{-1} + \lambda \right) \sum_{d_1,\ldots,d_{n-1}=1}^{\infty} A_1^{d_1} \ldots A_n^{d_n} \,|K; d_1, \ldots, d_n = 1\rangle \ .
\end{aligned}
\tag{B.9}
$$

We thus obtain n equations for the n parameters $A_1, \ldots, A_n$

$$
\begin{aligned}
e^{\mathrm{i}\frac{K}{n+1}} A_1^{-1} + e^{-\mathrm{i}\frac{K}{n+1}} A_1^{-1} A_2 + \lambda = 0 \\
e^{\mathrm{i}\frac{K}{n+1}} A_{m-1} A_m^{-1} + e^{-\mathrm{i}\frac{K}{n+1}} A_m^{-1} A_{m+1} + \lambda = 0 \\
e^{\mathrm{i}\frac{K}{n+1}} A_{n-1} A_n^{-1} + e^{-\mathrm{i}\frac{K}{n+1}} A_n^{-1} + \lambda = 0
\end{aligned}
\tag{B.10}
$$

for all $1 < m < n$. By multiplying the m-th equation with A_m we obtain a system of linear equations that can be written as

$$
\begin{pmatrix} e^{\mathrm{i}\frac{K}{n+1}} \\ 0 \\ \vdots \\ \vdots \\ 0 \\ e^{-\mathrm{i}\frac{K}{n+1}} \end{pmatrix} + M \begin{pmatrix} A_1 \\ A_2 \\ \vdots \\ \vdots \\ A_{n-1} \\ A_n \end{pmatrix} = \mathbf{0}
\tag{B.11}
$$

With the tri-diagonal Toplitz matrix

$$M = \begin{pmatrix} \lambda & e^{-\mathrm{i}\frac{K}{n+1}} & 0 & \cdots & \cdots & \cdots & \cdots & 0 \\ e^{\mathrm{i}\frac{K}{n+1}} & \lambda & e^{-\mathrm{i}\frac{K}{n+1}} & 0 & & & & \vdots \\ 0 & e^{\mathrm{i}\frac{K}{n+1}} & \lambda & e^{-\mathrm{i}\frac{K}{n+1}} & \ddots & & & \vdots \\ \vdots & 0 & \ddots & \ddots & \ddots & \ddots & & \vdots \\ \vdots & & \ddots & \ddots & \ddots & \ddots & 0 & \vdots \\ \vdots & & & \ddots & e^{\mathrm{i}\frac{K}{n+1}} & \lambda & e^{-\mathrm{i}\frac{K}{n+1}} & 0 \\ \vdots & & & & 0 & e^{\mathrm{i}\frac{K}{n+1}} & \lambda & e^{-\mathrm{i}\frac{K}{n+1}} \\ 0 & \cdots & \cdots & \cdots & \cdots & 0 & e^{\mathrm{i}\frac{K}{n+1}} & \lambda \end{pmatrix} . \quad \text{(B.12)}$$

Thus we obtain the result

$$\begin{pmatrix} A_1 \\ A_2 \\ \vdots \\ \vdots \\ A_{n-1} \\ A_n \end{pmatrix} = -M^{-1} \begin{pmatrix} e^{\mathrm{i}\frac{K}{n+1}} \\ 0 \\ \vdots \\ \vdots \\ 0 \\ e^{-\mathrm{i}\frac{K}{n+1}} \end{pmatrix} . \quad \text{(B.13)}$$

A normalisable bound-state exists if the parameters $A_1, ..., A_n$ for all m satisfy the condition

$$|A_m| < 1 . \quad \text{(B.14)}$$

The energy of the bound-state is given by

$$\begin{aligned} E_B &= e^{-\mathrm{i}\frac{K}{n+1}} \left(A_1 + \sum_{m=1}^{n-1} A_m^{-1} A_{m+1} + A_n^{-1} \right) + e^{+\mathrm{i}\frac{K}{n+1}} \left(A_1^{-1} + \sum_{m=1}^{n-1} A_m A_{m+1}^{-1} + A_n \right) = \\ &= -n\lambda + e^{-\mathrm{i}\frac{K}{n+1}} A_1 + e^{+\mathrm{i}\frac{K}{n+1}} A_n . \end{aligned} \quad \text{(B.15)}$$

We can plot the condition

$$|A_m| < 1 \ \forall m . \quad \text{(B.16)}$$

for general n-particle states. As shown in figure B.1 for two- to five-particle bound-states.

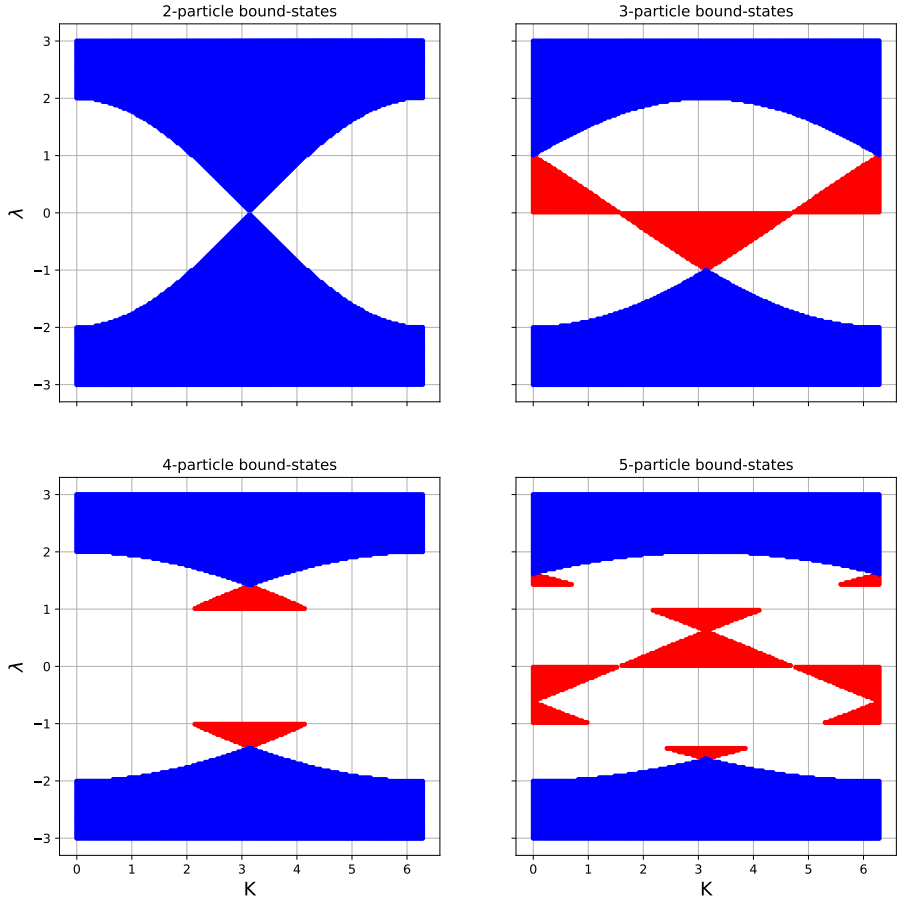

Figure B.1: Combination of nearest neighbour interaction strength λ and total momentum K for which bound-multi-particle states in the XXZ chain exist for two to five particles. The states coloured blue lie outside the continuum, states coloured red lie inside the continuum.

Note that for three and more particle bound-state with energies inside the continuum exist. These are normalisable states that can only exist inside the continuum due

to the conserved quantities of the integrable model. These bound-state inside the continuum are not stable under most perturbations, as most perturbations no longer conserve these conserved quantities. As an example we can introduce attractive density-density-density interactions

$$V_{ddd} = -\lambda_d \sum_i n_{i+2} n_{i+1} n_i \tag{B.17}$$

to the XXZ-chain and look at the three-particle sector. Intuitively this additional attractive interaction should only lower the energy of the three-particle bound-states, which is exactly what happens for bound-states with energies outside the continuum. Former bound-states inside the continuum are no longer stable though and become quasi-free states as this new interaction no longer conserves the conserved quantities of the integrable model that separated the bound-states and the quasi-free states inside the continuum. Figure B.2 depicts this phenomenon where we compare numerical diagonalisation results using the expectation value technique V.2 to compare the three-particle bound-states at total momentum $K = 0$ with and without the additional interaction.

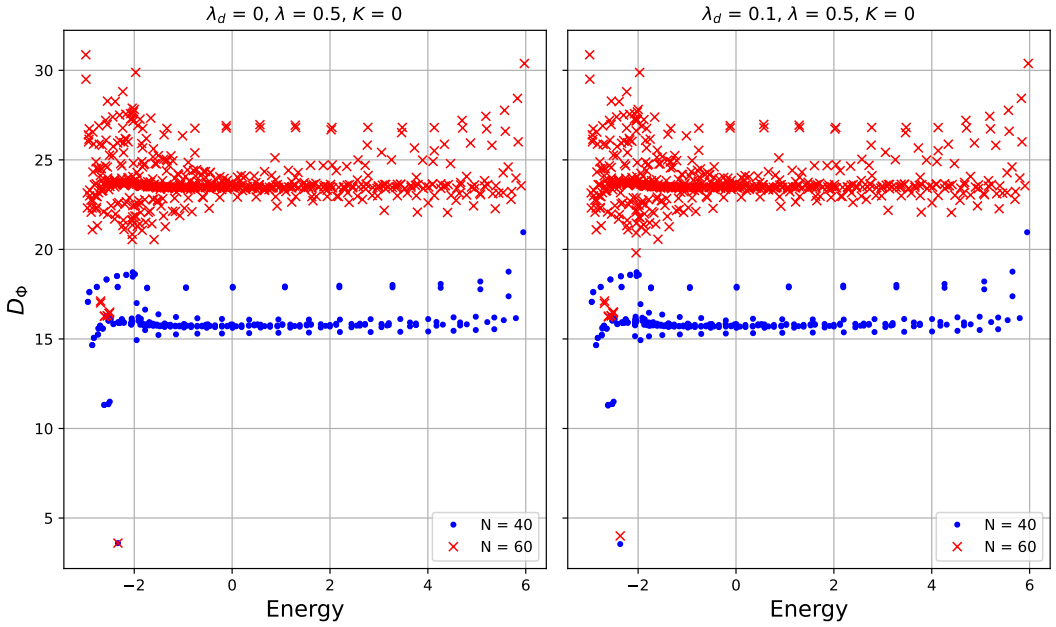

Figure B.2: Expectation value of the sum of distances between three particles in the one-dimensional XXZ model with and without attractive density-density-density interaction λ_d at fixed total momentum $K = 0$ and nearest neighbour interaction $\lambda = 0.5$ with periodic boundary conditions. The bound-state inside the continuum vanishes even though we only introduced attractive interaction as the density-density-density interaction does not conserved the conserved quantities of the integrable model.

C Three hard-core bosons on a one-dimensional chain with density-density-density interactions

We look at the simplest paradigmatic model which forms a bound three-particle state of hard-core bosons only due to genuine three-particle interactions

$$H_{\mathrm{ddd}} = \frac{1}{2}\sum_i a_{i+1}^\dagger a_i + \mathrm{h.c.} - \lambda_2 \sum_i n_{i+2} n_{i+1} n_i \tag{C.1}$$

with $n_i = a_i^\dagger a_i$ and hard-core boson operators $a_i^\dagger$, a_i.
We first apply a Jordan-Wigner transformation to fermionic operators

$$c_j^\dagger = a_j^\dagger e^{i\pi \sum_{l<j} n_l} \tag{C.2}$$

to obtain the transformed Hamiltonian

$$H_{\mathrm{ddd}} = \frac{1}{2}\sum_i c_{i+1}^\dagger c_i + \mathrm{h.c.} - \lambda_2 \sum_i n_{i+2}^c n_{i+1}^c n_i^c \tag{C.3}$$

with $n_i^c = c_i^\dagger c_i$.
We now split the Hamiltonian into a free and interacting part

$$\begin{aligned} H_{\mathrm{ddd}} &= H_0 + V \\ H_0 &= \sum_i c_{i+1}^\dagger c_i + \mathrm{h.c.} \\ V &= -\lambda_2 \sum_i n_{i+2}^c n_{i+1}^c n_i^c \ . \end{aligned} \tag{C.4}$$

The eigenstates of the free Hamiltonian in the three-particle sector are readily given in fermionic language

$$
\begin{aligned}
c_k^\dagger &= \frac{1}{\sqrt{N}} \sum_j e^{ijk} c_j^\dagger \\
|k_1, k_2, k_3\rangle &= c_{k_1}^\dagger c_{k_2}^\dagger c_{k_3}^\dagger |0\rangle \\
H_0 |k_1, k_2, k_3\rangle &= \omega(k_1, k_2, k_3) |k_1, k_2, k_3\rangle \\
\omega(k_1, k_2, k_3) &= \cos(k_1) + \cos(k_2) + \cos(k_3) \ .
\end{aligned}
\tag{C.5}
$$

We can write down the corresponding free Green's function

$$
G_0(z) = \frac{1}{6} \sum_{k_1,k_2,k_3} \frac{|k_1, k_2, k_3\rangle \langle k_1, k_2, k_3|}{z - \omega(k_1, k_2, k_3)} \tag{C.6}
$$

where the factor $1/6 = 1/3!$ prevents double counting and define a (K,d) basis, which exploits the fact that the interaction Hamiltonian is merely a projection operator for fixed total momenta K

$$
|K; d_1, d_2\rangle = \frac{1}{\sqrt{N}} \sum_j e^{ijK} c_j^\dagger c_{j+d_1}^\dagger c_{j+d_1+d_2}^\dagger |0\rangle \tag{C.7}
$$

with $d_1, d_2 > 0$. In this basis we find

$$
V |K; d_1, d_2\rangle = -\lambda_2 \delta_{d_1,1} \delta_{d_2,1} |K; d_1, d_2\rangle \ . \tag{C.8}
$$

We can now use the Green's function method to obtain a implicit formula for the bound-state energy ϵ_{Bound}

$$
\mathbf{det} \left(1 - V G_0(\epsilon_{\text{Bound}}) P\right) = 0 \ . \tag{C.9}
$$

For a fixed total momentum K the image of the interaction V is only one dimensional spanned by $|K; 1, 1\rangle$. The above equation thus reduces to

$$
0 = 1 + \frac{\lambda_2}{6} \sum_{k_1,k_2,k_3} \frac{|\langle K; 1, 1|k_1, k_2, k_3\rangle|^2}{\epsilon_{\text{Bound}}^{(3)}(K) - \omega(k_1, k_2, k_3)} \ . \tag{C.10}
$$

The overlap between the two basis vectors is given by

$$
\begin{aligned}
|\langle K; 1, 1|k_1, k_2, k_3\rangle|^2 = \delta_{K,k_1+k_2+k_3} \frac{16}{N} \sin^2\left(\frac{k_1 - k_2}{2}\right) \times \\
\times \left(\cos\left(K - \frac{3}{2}(k_1 + k_2)\right) - \cos\left(\frac{k_1 - k_2}{2}\right)\right)^2 \ .
\end{aligned}
\tag{C.11}
$$

The implicit equation can be written in the continuum limit as

$$f(z = \epsilon^{(3)}_{\text{Bound}}(K), K) = 1 + \frac{2\lambda_2}{3\pi^2} I(\epsilon^{(3)}_{\text{Bound}}(K), K) = 0$$
$$I(z, K) = \int_0^{2\pi} \int_0^{2\pi} \frac{\sin^2\left(\frac{k_1-k_2}{2}\right)\left(\cos\left(K - \frac{3}{2}(k_1+k_2)\right) - \cos\left(\frac{k_1-k_2}{2}\right)\right)^2}{z - (\cos(k) + \cos(k') + \cos(K-k-k'))} dk\, dk' \,. \tag{C.12}$$

The implicit function is bound in the limit that z approaches the lower bound of the continuum (see figure C.1). This corresponds to the case that a bound state exists only for $\lambda_2 > \lambda_c > 0$. The lower bound of the continuum lies at an energy of $-3/2$ at $K = 0$. The corresponding momentum values are $(k, k') = (2\pi/3, 2\pi/3)$, so for $z = -3/2$ the denominator in the integral $I(z = -3/2, K = 0)$ diverges, but the numerator of the fraction also tends to zero, in such a way that the integral is still defined. We can thus determine the critical value of the density-density-density interaction for which a bound-state exists at all values of the total momentum K via

$$\lambda_c = -\frac{3\pi^2}{2I(-3/2, 0)} \approx 1.173222 \,. \tag{C.13}$$

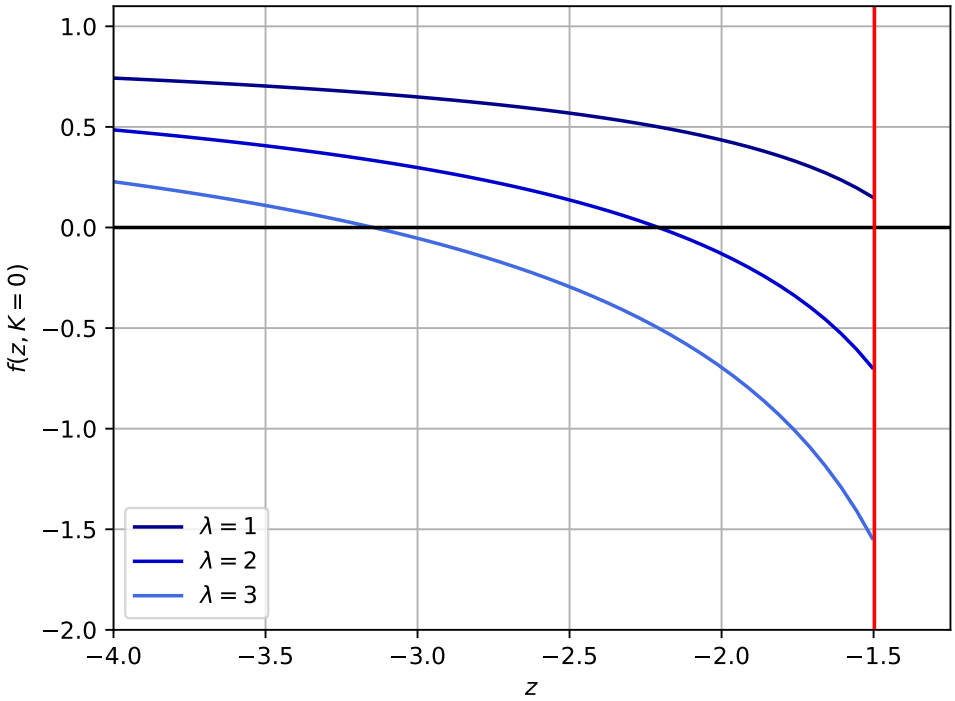

Figure C.1: Implicit function $f(z, \lambda_2, K)$ of the one dimensional chain with density-density-density interaction for total momentum $K = 0$ and a range of interaction strengths λ_2. A root and thus a bound-state is only present for $\lambda_2 < \lambda_c = 1.173$.

D Two-particle bound-state energies of two long-range XXZ models in one dimension

D.1 One-dimensional discrete Hydrogen atom

We will study the XXZ-chain with long-range interaction of the form

$$H = \frac{1}{2}\sum_i a_{i+1}^\dagger a_i + \text{h.c.} - V\sum_i \sum_{d=1}^{\infty} \frac{1}{d} n_{i+d} n_i \tag{D.1}$$

the interaction strength $\lambda(d) = V/d$ with $V > 0$ decays as $1/\text{distance}$ which we will call Coulomb-like. We want to study the formation of two-particle bound-states between two hard-core bosons and will show that analytical expressions for all bound-states and their energies can be obtained using the recursion ansatz discussed in chapter VI.2. These results have already be calculated in [14].
Using the recursion relations discussed in (VI.99) we find for this model

$$\begin{aligned} H|\Psi\rangle &= \epsilon|\Psi\rangle \\ \epsilon g(1) &= \cos(K/2)g(2) - Vg(1) \\ \epsilon g(d) &= \cos(K/2)\left(g(d+1) + g(d-1)\right) - \frac{V}{d}g(d) \end{aligned} \tag{D.2}$$

for $d > 1$. Without loss of generality we will choose $g(1) = 1$ thus giving

$$g(2) = \frac{\epsilon + V}{\cos(K/2)} \,. \tag{D.3}$$

The goal is to solve this recursive equation and identify the eigenvalues by the condition that $|\Psi\rangle$ is normalizable, i.e.

$$\sum_{d=1}^{\infty} |g(d)|^2 < \infty \tag{D.4}$$

D.1.1 Solving the recursive equation using generating functions

We start by defining a function as a formal power series using the coefficients of our eigenvector $g(d)$ as

$$F(x) = \sum_{d=1}^{\infty} g(d)x^d = x + \sum_{d=2}^{\infty} g(d)x^d = x + \tilde{F}(x) \tag{D.5}$$

here we already used $g(1) = 1$. We can now use the eigenvalue equation (D.2) for $d > 1$ to rewrite $\tilde{F}(x)$ as

$$\begin{aligned}
\epsilon\tilde{F}(x) &= \sum_{d=2}^{\infty} \epsilon g(d)x^d = \\
&= \sum_{d=2}^{\infty} \left(\cos(K/2)\left(g(d+1) + g(d-1)\right) - \frac{V}{d}g(d) \right) x^d = \\
&= \cos(K/2)\left(\frac{1}{x}\left(\tilde{F}(x) - g(2)x^2\right) + x\left(\tilde{F}(x) + x\right)\right) - VL(x) = \\
&= \cos(K/2)\left(\left(x + \frac{1}{x}\right) F(x) - \frac{\epsilon + V}{\cos(K/2)}x - 1 \right) - VL(x)
\end{aligned} \tag{D.6}$$

where we defined the function

$$L(x) = \sum_{d=2}^{\infty} \frac{1}{d} g(d)x^d \ . \tag{D.7}$$

We can now solve for the generating function $F(x)$ as

$$\left(\epsilon - \cos(K/2)\left(x + \frac{1}{x}\right)\right) F(x) = -\cos(K/2) - Vx - VL(x) \ . \tag{D.8}$$

We now note that $F(x)$ and $L(x)$ are related via their derivative

$$L'(x) = \sum_{d=2}^{\infty} g(d)x^{d-1} = \frac{1}{x}\left(F(x) - x\right) \ . \tag{D.9}$$

We define the helper function

$$h(x) = \epsilon - \cos(K/2)\left(x + \frac{1}{x}\right) \tag{D.10}$$

and differentiate equation (D.8) to obtain a linear differential equation for the generating function

$$\begin{aligned} h'(x)F(x) + h(x)F'(x) &= -V - VL'(x) \\ h'(x)F(x) + h(x)F'(x) &= -V - V\left(\frac{1}{x}F(x) - 1\right) = -\frac{V}{x}F(x) \\ \left(h'(x) + \frac{V}{x}\right)F(x) &= -h(x)F'(x) \\ \frac{F'(x)}{F(x)} &= -\frac{h'(x) + V/x}{h(x)} = -\frac{h'(x)}{h(x)} + -\frac{V}{xh(x)} \ . \end{aligned} \tag{D.11}$$

The function $xh(x)$ is just a quadratic polynomial. We will factorise this as

$$\begin{aligned} xh(x) &= -\cos(K/2)\left(x^2 - \frac{\epsilon}{\cos(K/2)}x + 1\right) \\ x^2 - \frac{\epsilon}{\cos(K/2)}x + 1 &= (x - x_1)(x - x_2) \\ x_{1/2} &= \frac{\epsilon}{2\cos(K/2)} \pm \sqrt{\left(\frac{\epsilon}{2\cos(K/2)}\right)^2 - 1} \\ xh(x) &= -\cos(K/2)(x - x_1)(x - x_2) \\ \frac{1}{xh(x)} &= \frac{1}{\cos(K/2)\,(x_2 - x_1)}\left(\frac{1}{x - x_1} - \frac{1}{x - x_2}\right) \end{aligned} \tag{D.12}$$

where in the last step we performed a partial fraction decomposition. With this we can solve the differential equation (D.11) by integration

$$\begin{aligned} \frac{F'(x)}{F(x)} &= -\frac{h'(x) + V/x}{h(x)} = -\frac{h'(x)}{h(x)} + \frac{V}{\cos(K/2)\,(x_1 - x_2)}\left(\frac{1}{x - x_1} - \frac{1}{x - x_2}\right) \\ \ln(F(x)) &= -\ln(h(x)) + \frac{V}{\cos(K/2)\,(x_1 - x_2)}\left(\ln(x - x_1) - \ln(x - x_2)\right) + \tilde{C} \\ F(x) &= C\frac{1}{h(x)}\left(\frac{x - x_1}{x - x_2}\right)^{\alpha} \\ \alpha &= \frac{V}{\cos(K/2)\,(x_1 - x_2)} = \frac{V}{2\cos(K/2)\sqrt{\left(\frac{\epsilon}{2\cos(K/2)}\right)^2 - 1}} \end{aligned} \tag{D.13}$$

We can fix the integration constant C by the condition $g(1) = 1$, i.e. $F'(0) = 1$

$$
\begin{aligned}
F'(0) &= -C\left(\frac{x_1}{x_2}\right)^{\alpha} \lim_{x\to 0} \frac{h'(x)}{h^2(x)} + \frac{V}{xh^2(x)} = \\
&= -C\left(\frac{x_1}{x_2}\right)^{\alpha} \lim_{x\to 0} \frac{x^2 h'(x)}{(xh(x))^2} = -C\left(\frac{x_1}{x_2}\right)^{\alpha} \frac{1}{\cos(K/2)} \qquad \text{(D.14)} \\
C &= -\cos(K/2)\left(\frac{x_2}{x_1}\right)^{\alpha} .
\end{aligned}
$$

Thus the full generating function is given by

$$
F(x) = \frac{x}{(x-x_1)(x-x_2)}\left(\frac{1-x/x_1}{1-x/x_2}\right)^{\alpha} . \qquad \text{(D.15)}
$$

For every value of ϵ the coefficients of the series expansion of $F(x)$ around $x = 0$ yield an 'eigenvector' with 'eigenvalue' ϵ. This yield an uncountable number of solutions which have to be reduced to a finite or countably infinite number of solution by demanding the normalisablity of these states.

D.1.2 Finding the normalisable solutions from the generating function

The simplest approach to study the convergence of the potential eigenstates is to obtain an explicit formula for them. We therefore expand the generating function (D.15) around $x = 0$. First we rewrite the generating function as

$$
F(x) = \frac{x}{x_1 x_2}\left(1-x/x_1\right)^{\alpha-1}\left(1-x/x_2\right)^{-\alpha-1} . \qquad \text{(D.16)}
$$

Next we use the generalised binomial formula

$$
(1+x)^{\alpha} = \sum_{n=0}^{\infty} \binom{\alpha}{n} x^n \qquad \text{(D.17)}
$$

with the generalised binomial coefficient with general $\alpha \in \mathbb{C}$. Thus we get

$$
\begin{aligned}
F(x) &= \frac{x}{x_1 x_2}\left(1 - x/x_1\right)^{\alpha-1}\left(1 - x/x_2\right)^{-\alpha-1} \\
&= \frac{x}{x_1 x_2}\sum_{k=0}^{\infty}\sum_{l=0}^{\infty}(-1)^{k+l}\binom{\alpha-1}{k}\binom{-\alpha-1}{l}\frac{1}{x_1^k}\frac{1}{x_2^l}x^{k+l} = \\
&= \frac{x}{x_1 x_2}\sum_{n=0}^{\infty}(-1)^n x^n \sum_{m=0}^{n}\binom{\alpha-1}{m}\binom{-\alpha-1}{n-m}\frac{1}{x_1^m}\frac{1}{x_2^{n-m}} = \\
&= \frac{x}{x_1 x_2}\sum_{n=0}^{\infty}(-1)^n\binom{-\alpha-1}{n}\frac{1}{x_2^n}{}_2F_1(1-\alpha,-n;-\alpha-n;\frac{x_2}{x_1})x^n
\end{aligned}
\tag{D.18}
$$

Here ${}_2F_1(a,b;c;z)$ denotes the Hypergeometric function. Thus we can identify the components of the eigenvectors as

$$
g(d) = (-1)^{d-1}\binom{-\alpha-1}{d-1}{}_2F_1(1-\alpha,-d+1;-\alpha-d+1;\frac{x_2}{x_1})\frac{1}{x_2^{d-1}}\ . \tag{D.19}
$$

We now need to identify the possible eigenvalues that yield normalisable eigenvectors. First we note that $x_1 x_2 = 1$ and that $|x_2| > 1$ for $\epsilon < 0$. We also note that the Hypergeometric function $F_1(1-\alpha,-d+1;-\alpha-d+1;\frac{x_2}{x_1})$ reduces to a finite polynomial in $\frac{x_2}{x_1} = x_2^2$ of order $d-1$, thus we find that

$$
{}_2F_1(1-\alpha,-d+1;-\alpha-d+1;x_2^2)\frac{1}{x_2^{d-1}} \tag{D.20}
$$

is a power series in x_2 with powers ranging between $-(d-1)$ and $d-1$. Since $|x_2| > 1$ the positive powers of x_2 that scale with d make the state non-normalisable. Therefore the Hypergeometric function must not only be a finite polynomial of degree $x_2^{2(d-1)}$ but of some maximal power $x_2^{d_{\max}}$ for all large values of d. A Hypergeometric function ${}_2F_1(a,b;c;z)$ reduces to a finite polynomial if either a or b are negative integers. b is always a negative integer given by $-(d-1)$. If we want only a maximal power in the Hypergeometric function independent of d we need $a = 1-\alpha$ to be a negative integer including zero. The normalisation condition is thus given by

$$
\begin{aligned}
\alpha &= m \in \mathbb{N}/\{0\} \\
m &= \frac{V}{\sqrt{\epsilon^2 - 4\cos^2(K/2)}} \\
\epsilon &= \pm\sqrt{\left(\frac{V}{m}\right)^2 + 4\cos^2(K/2)}\ .
\end{aligned}
\tag{D.21}
$$

Note that we required $\epsilon < 0$ thus only the negative solution yields physically acceptable states.
With this we can summaries our results.
The long-range-Coulomb-XXZ chain displays an infinite amount of bound-states labelled by a non-zero integer quantum number m with eigenenergies

$$\epsilon_{\text{bound}}(m) = -\sqrt{\left(\frac{V}{m}\right)^2 + 4\cos^2(K/2)} \tag{D.22}$$

and corresponding eigenvectors

$$\begin{aligned} |\Psi\rangle &= \sum_{d=1}^{\infty} g_m(d)\,|K;d\rangle \\ g_m(d) &= (-1)^{d-1}\binom{-m-1}{d-1}\,{}_2F_1(1-m,-d+1;-m-d+1;x_2^2)\frac{1}{x_2^{d-1}} \\ x_2 &= \frac{1}{2\cos(K/2)}\left(\epsilon_{\text{bound}}(m) - \sqrt{\epsilon_{\text{bound}}^2(m) - 4\cos^2(K/2)}\right)\ . \end{aligned} \tag{D.23}$$

Note that these results only hold for $V > 0$.

D.2 The long-range exponential decay XXZ chain

We will now study the bound-states in the XXZ chain with exponentially decaying long-range interactions

$$H = \frac{1}{2}\sum_i a_{i+1}^\dagger a_i + \text{h.c.} - V\sum_i\sum_{d=1}^{\infty}\alpha^{d-1}n_{i+d}n_i \tag{D.24}$$

with $V > 0$ and $\alpha < 1$. We again make the general ansatz in the (K,d)-Basis leading to the following set of eigen-equations

$$\begin{aligned} H\,|\Psi\rangle &= \epsilon\,|\Psi\rangle \\ \epsilon g(1) &= \cos(K/2)g(2) - Vg(1) \\ \epsilon g(d) &= \cos(K/2)\left(g(d+1) + g(d-1)\right) - \frac{V}{\alpha}\alpha^d g(d) \end{aligned} \tag{D.25}$$

for $d > 1$. Without loss of generality we will choose $g(1) = 1$ thus giving

$$g(2) = \frac{\epsilon + V}{\cos(K/2)} g(1) \ . \tag{D.26}$$

D.2.1 Solving the recursive equation using generating functions

We can define a generating function analogously to the section beforehand

$$F(x) = \sum_{d=1}^{\infty} g(d) x^d = x + \sum_{d=2}^{\infty} g(d) x^d = x + \tilde{F}(x) \tag{D.27}$$

here we already used $g(1) = 1$. We can now use the eigenvalue equation (VI.97) for $d > 1$ to rewrite $\tilde{F}(x)$ as

$$\begin{aligned}
\epsilon \tilde{F}(x) &= \sum_{d=2}^{\infty} \epsilon g(d) x^d = \\
&= \sum_{d=2}^{\infty} \left(\cos(K/2) \left(g(d+1) + g(d-1) \right) - \frac{V}{\alpha} \alpha^d g(d) \right) x^d = \\
&= \cos(K/2) \left(\frac{1}{x} \left(\tilde{F}(x) - g(2) x^2 \right) + x \left(\tilde{F}(x) + x \right) \right) - \frac{V}{\alpha} L(x) = \\
&= \cos(K/2) \left(\left(x + \frac{1}{x} \right) F(x) - \frac{\epsilon + V}{\cos(K/2)} x - 1 \right) - \frac{V}{\alpha} L(x)
\end{aligned} \tag{D.28}$$

where we defined the function

$$L(x) = \sum_{d=2}^{\infty} g(d) \alpha^d x^d \ . \tag{D.29}$$

We can now solve for the generating function $F(x)$ as

$$\left(\epsilon - \cos(K/2) \left(x + \frac{1}{x} \right) \right) F(x) = -\cos(K/2) - Vx - \frac{V}{\alpha} L(x) \ . \tag{D.30}$$

This time around $L(x)$ and $F(x)$ are no longer related via their derivative instead we find the functional connection

$$L(x) = F(\alpha x) - \alpha x \ . \tag{D.31}$$

With this we obtain the characteristic equation for our generating function

$$h(x)F(x) = F(\alpha x) + c \tag{D.32}$$

with the functions

$$\begin{aligned} h(x) &= -\frac{\alpha}{V}\left(\epsilon - \cos(K/2)\left(x + \frac{1}{x}\right)\right) = \frac{\alpha\cos(K/2)}{Vx}(x - x_1)(x - x_2) \\ c &= \frac{\alpha\cos(K/2)}{V} \ . \end{aligned} \tag{D.33}$$

This time instead of a linear differential equation we have to solve the functional equation (D.32) to obtain the generating function for our problem.

In order to find a solution to our equation we will consider the simpler functional equation

$$F(\alpha x) = h(x)F(x) \tag{D.34}$$

first. Note that the function $h(x)$ is not the actual function of our problem but a place holder!

We find

$$\begin{aligned} F(\alpha^2 x) &= F(\alpha(\alpha x)) = h(\alpha x)F(\alpha x) = h(\alpha x)h(x)F(x) \\ F(\alpha^n x) &= F(x)\prod_{j=0}^{n-1} h(\alpha^j x) \\ F(0) &= \lim_{n\to\infty} F(\alpha^n x) = F(x)\prod_{j=0}^{\infty} h(\alpha^j x) \\ F(x) &= \frac{F(0)}{\prod_{j=0}^{\infty} h(\alpha^j x)} \ . \end{aligned} \tag{D.35}$$

Now similar to variation of the constant in the theory of differential equations we will make the ansatz

$$F(x) = \frac{r(x)}{\prod_{j=0}^{\infty} h(\alpha^j x)} \tag{D.36}$$

for the full functional equation (D.32) and we find

$$
\begin{aligned}
F(\alpha x) &= h(x)\frac{r(\alpha x)}{\prod_{j=0}^{\infty} h(\alpha^j x)} \\
h(x)F(x) - c &= h(x)\frac{r(x)}{\prod_{j=0}^{\infty} h(\alpha^j x)} - c \\
r(\alpha x) &= r(x) - \frac{\prod_{j=0}^{\infty} h(\alpha^j x)}{h(x)}c \\
r(\alpha^2 x) &= r(\alpha(\alpha x)) = r(\alpha x) - \frac{\prod_{j=0}^{\infty} h(\alpha^j x)}{h(\alpha x)h(x)}c = \\
&= r(x) - \frac{\prod_{j=0}^{\infty} h(\alpha^j x)}{h(x)}c - \frac{\prod_{j=0}^{\infty} h(\alpha^j x)}{h(\alpha x)h(x)}c \\
r(\alpha^n x) &= r(x) - c\sum_{m=0}^{n-1}\frac{\prod_{j=0}^{\infty} h(\alpha^j x)}{\prod_{j=0}^{m} h(\alpha^j x)} \\
r(0) &= \lim_{n\to\infty} r(\alpha^n x) = r(x) - c\sum_{m=0}^{\infty}\frac{\prod_{j=0}^{\infty} h(\alpha^j x)}{\prod_{j=0}^{m} h(\alpha^j x)} \\
r(x) &= r(0) + c\sum_{m=0}^{\infty}\frac{\prod_{j=0}^{\infty} h(\alpha^j x)}{\prod_{j=0}^{m} h(\alpha^j x)} \\
F(x) &= \frac{r(0)}{\prod_{j=0}^{\infty} h(\alpha^j x)} + c\sum_{m=0}^{\infty}\frac{1}{\prod_{j=0}^{m} h(\alpha^j x)} \ .
\end{aligned}
\tag{D.37}
$$

We note two things to this solution.
First we do not now if this is the unique solution to the functional equation.
Second for our specific choice of $h(x)$ the infinite product $\prod_{j=0}^{\infty} h(\alpha^j x)$ is ill defined at all values of x.
It turns out that the case $r(0) = 0$ and the solution

$$
F(x) = c\sum_{m=0}^{\infty}\frac{1}{\prod_{j=0}^{m} h(\alpha^j x)} \tag{D.38}
$$

satisfies the condition $F'(0) = 1$ (this fact will become apparent later) and is well defined for sufficiently small values of x. We will thus take (D.38) as the solution for our generating function. We will now simplify this expression using

$$\begin{aligned}\prod_{j=0}^{m} h(\alpha^j x) &= \prod_{j=0}^{m} \frac{\alpha\cos(K/2)}{V\alpha^j x}(\alpha^j x - x_1)(\alpha^j x - x_2) = \\ &= \left(\frac{\alpha\cos(K/2)}{Vx}\right)^{m+1} \alpha^{-(m+1)m/2} \prod_{j=0}^{m}\left(1-\frac{x}{x_1}\alpha^j\right)\left(1-\frac{x}{x_2}\alpha^j\right) = \\ &= \left(\frac{\cos(K/2)}{Vx}\right)^{m+1} \alpha^{-(m+1)(m-2)/2}\left(\frac{x}{x_1};\alpha\right)_{m+1}\left(\frac{x}{x_2};\alpha\right)_{m+1}\end{aligned} \tag{D.39}$$

where we used the q-Pochhammer symbol

$$(a;q)_m = \prod_{j=0}^{m-1}\left(1-aq^j\right) \ . \tag{D.40}$$

The q-Pochhammer symbol enjoys a number of useful identities so we find

$$\begin{aligned}\frac{1}{(a;q)_m} &= \frac{(q^m a;q)_\infty}{(a;q)_\infty} \\ \frac{(ax;q)_\infty}{(x;q)_\infty} &= \sum_{n=0}^{\infty}\frac{(a;q)_n}{(q;q)_n}x^n \\ \frac{1}{(x;\alpha)_m} &= \frac{(\alpha^m x;\alpha)_\infty}{(x;\alpha)_\infty} = \sum_{n=0}^{\infty}\frac{(\alpha^m;\alpha)_n}{(\alpha;\alpha)_n}x^n \ .\end{aligned} \tag{D.41}$$

With this we find the expansion

$$\frac{1}{\left(\frac{x}{x_{1/2}};\alpha\right)_{m+1}} = \sum_{n=0}^{\infty}\frac{(\alpha^{m+1};\alpha)_n}{(\alpha;\alpha)_n}\left(\frac{x}{x_{1/2}}\right)^n \tag{D.42}$$

and thus

$$\begin{aligned}
\frac{1}{\left(\frac{x}{x_1};\alpha\right)_{m+1}\left(\frac{x}{x_2};\alpha\right)_{m+1}} &= \sum_{l=0}^{\infty}\sum_{n=0}^{\infty}\frac{\left(\alpha^{m+1};\alpha\right)_l}{\left(\alpha;\alpha\right)_l}\frac{\left(\alpha^{m+1};\alpha\right)_n}{\left(\alpha;\alpha\right)_n}\left(\frac{x}{x_1}\right)^l\left(\frac{x}{x_2}\right)^n = \\
&= \sum_{n=0}^{\infty} b_n^m(\alpha)x^n \\
b_n^m(\alpha) &= \sum_{l=0}^{n}\frac{\left(\alpha^{m+1};\alpha\right)_l}{\left(\alpha;\alpha\right)_l}\frac{\left(\alpha^{m+1};\alpha\right)_{n-l}}{\left(\alpha;\alpha\right)_{n-l}}\frac{1}{x_1^l}\frac{1}{x_2^{n-l}} = \\
&= \frac{1}{x_2^n}\sum_{l=0}^{n}\frac{\left(\alpha^{m+1};\alpha\right)_l}{\left(\alpha;\alpha\right)_l}\frac{\left(\alpha^{m+1};\alpha\right)_{n-l}}{\left(\alpha;\alpha\right)_{n-l}}x_2^{2l} = \\
&= \frac{\left(\alpha^{m+1};\alpha\right)_n}{\left(\alpha;\alpha\right)_n}\frac{1}{x_2^n}{}_2\phi_1\left(\alpha^{m+1},\alpha^{-n};\alpha^{-(n+m)};\alpha,\alpha^{-m}x_2^2\right) .
\end{aligned} \tag{D.43}$$

Where we used the basic hypergeometric function

$${}_2\phi_1(a,b;c;q,z) = \sum_{l=0}^{\infty}\frac{(a;q)_l\,(b;q)_l}{(c;q)_l}\frac{z^l}{(q;q)_l} . \tag{D.44}$$

We can reinsert all these expressions into our generating function (D.38) to obtain

$$\begin{aligned}
F(x) &= c\sum_{n,m=0}^{\infty}\left(\frac{Vx}{\cos(K/2)}\right)^{m+1}\alpha^{(m+1)(m-2)/2}b_n^m(\alpha)x^n \\
&= xc\sum_{n,m=0}^{\infty}\left(\frac{V}{\cos(K/2)}\right)^{m+1}\alpha^{(m+1)(m-2)/2}b_n^m(\alpha)x^{n+m} = \\
&= x\sum_{n=0}^{\infty} l_1(n)x^n
\end{aligned} \tag{D.45}$$

with

$$l_1(n) = \sum_{m=0}^{n}\left(\frac{V}{\cos(K/2)}\right)^m\alpha^{m(m-1)/2}b_{n-m}^m(\alpha) . \tag{D.46}$$

So we find

$$F(x) = x \sum_{n=1}^{\infty} l_1(n) x^n \ . \tag{D.47}$$

We can finally identify the coefficients of our series as

$$g(d) = l_1(d-1) \ . \tag{D.48}$$

From this point it is easy to verify that $g(1) = 1$. Using these results we now have to identify the normalisable solutions for $g(d)$. The full expression for $g(d+1)$ is given by

$$\begin{aligned} g(d+1) = l_1(d) &= \sum_{m=0}^{d} \left(\frac{V}{\cos(K/2)}\right)^m \alpha^{m(m-1)/2} b_{d-m}^m(\alpha) = \\ &= \sum_{m=0}^{d} \left(\frac{V}{\cos(K/2)}\right)^m \alpha^{m(m-1)/2} \frac{\left(\alpha^{m+1};\alpha\right)_{d-m}}{(\alpha;\alpha)_{d-m}} \frac{1}{x_2^{d-m}} \times \\ &\times {}_2\phi_1\left(\alpha^{m+1}, \alpha^{-(d-m)}; \alpha^{-d}; \alpha, \alpha^{-m} x_2^2\right) = \\ &= \frac{1}{x_2^d} \sum_{m=0}^{d} \alpha^{m(m-1)/2} \frac{\left(\alpha^{m+1};\alpha\right)_{d-m}}{(\alpha;\alpha)_{d-m}} \left(\frac{V}{\cos(K/2)} x_2\right)^m \times \\ &\times {}_2\phi_1\left(\alpha^{m+1}, \alpha^{-(d-m)}; \alpha^{-d}; \alpha, \alpha^{-m} x_2^2\right) \end{aligned} \tag{D.49}$$

We notice that this time around it is not possible to choice ϵ (i.e. x_2) in such a way that the positive powers of x_2 do not grow like d. Thus we need another mechanism by which the coefficients $g(d+1)$ stay bounded. Notice the structure

$$g(d+1) = \frac{1}{x_2^d} P_d(x_2) \tag{D.50}$$

where $P_d(x_2)$ is a polynomial of order $2d$ in the variable x_2. For the normalisability of $g(d)$ it is a necessary condition that $\lim_{d\to\infty} g(d) = 0$. It is clear from the previous equation that this limit is not true for arbitrary values of x_2 as $P_d(x_2)$ is a polynomial of order $2d$ and the prefactor only vanishes like $1/x_2^d$. Thus the only way that $g(d)$ can vanish in the limit $d \to \infty$ for a fixed value of x_2 is, if $\lim_{d\to\infty} P_d(x_2) = 0$. For arbitrary large values of $|x_2| > 1$ the limit $\lim_{d\to\infty} P_d(x_2)$ is either $\pm\infty$. To obtain a limiting polynomial anyway we look at the ratio $g(d+1)/x_2^d$ instead as this converges in the limit $d \to \infty$ to a power series in $1/x_2$

$$\frac{g(d+1)}{x_2^d} = \frac{1}{x_2^{2d}} \sum_{m=0}^{d} \alpha^{m(m-1)/2} \frac{\left(\alpha^{m+1};\alpha\right)_{d-m}}{\left(\alpha;\alpha\right)_{d-m}} \left(\frac{V}{\cos(K/2)} x_2\right)^m \times \\ \times {}_2\phi_1\left(\alpha^{m+1}, \alpha^{-(d-m)}; \alpha^{-d}; \alpha, \alpha^{-m} x_2^2\right) . \tag{D.51}$$

We now have to find the limiting power series in $1/x_2$ in the limit $d \to \infty$ and determine its roots, thus fixing x_2 and the eigenvalues of our problem.

We start with the following manipulations

$$\frac{g(d+1)}{x_2^d} = \sum_{m=0}^{d} \alpha^{m(m-1)/2} \frac{\left(\alpha^{m+1};\alpha\right)_{d-m}}{\left(\alpha;\alpha\right)_{d-m}} \left(\frac{V}{\cos(K/2) x_2}\right)^m \times \\ \times \frac{1}{x_2^2}^{d-m} {}_2\phi_1\left(\alpha^{m+1}, \alpha^{-(d-m)}; \alpha^{-d}; \alpha, \alpha^{-m} x_2^2\right) . \tag{D.52}$$

Now we take a closer look at the expression

$$\begin{aligned} &\left(\frac{1}{x_2^2}\right)^{d-m} {}_2\phi_1\left(\alpha^{m+1}, \alpha^{-(d-m)}; \alpha^{-d}; \alpha, \alpha^{-m} x_2^2\right) = \\ &\quad = \sum_{l=0}^{d-m} \frac{\left(\alpha^{m+1};\alpha\right)_l \left(\alpha^{-(d-m)};\alpha\right)_l}{\left(\alpha^{-d};\alpha\right)_l \left(\alpha;\alpha\right)_l} \alpha^{-ml} \left(x_2^2\right)^{l-(d-m)} = \\ &\quad = \sum_{u=0}^{d-m} \frac{\left(\alpha^{m+1};\alpha\right)_{d-m-u} \left(\alpha^{-(d-m)};\alpha\right)_{d-m-u}}{\left(\alpha^{-d};\alpha\right)_{d-m-u} \left(\alpha;\alpha\right)_{d-m-u}} \alpha^{-m(d-m-u)} \left(\frac{1}{x_2^2}\right)^u = \\ &\quad = \sum_{u=0}^{d-m} \frac{\left(\alpha^{m+1};\alpha\right)_u \left(\alpha^{-(d-m)};\alpha\right)_u}{\left(\alpha^{-d};\alpha\right)_u \left(\alpha;\alpha\right)_u} \alpha^{-mu} \left(\frac{1}{x_2^2}\right)^u = \\ &\quad = {}_2\phi_1\left(\alpha^{m+1}, \alpha^{-(d-m)}; \alpha^{-d}; \alpha, \alpha^{-m} \frac{1}{x_2^2}\right) . \end{aligned} \tag{D.53}$$

We thus get the relation

$$\frac{g(d+1)}{x_2^d} = \sum_{m=0}^{d} \alpha^{m(m-1)/2} \frac{\left(\alpha^{m+1};\alpha\right)_{d-m}}{\left(\alpha;\alpha\right)_{d-m}} \left(\frac{V}{\cos(K/2) x_2}\right)^m \times \\ \times {}_2\phi_1\left(\alpha^{m+1}, \alpha^{-(d-m)}; \alpha^{-d}; \alpha, \alpha^{-m} \frac{1}{x_2^2}\right) . \tag{D.54}$$

We can now take the limit $d \to \infty$. We use the relations

$$\begin{aligned}\lim_{d\to\infty} {}_2\phi_1\left(\alpha^{m+1}, \alpha^{-(d-m)}; \alpha^{-d}; \alpha, \alpha^{-m}\frac{1}{x_2^2}\right) &= {}_1\phi_0\left(\alpha^{m+1}; -; \alpha, \frac{1}{x_2^2}\right) = \\ &= \frac{\left(\frac{a^{m+1}}{x_2^2}; \alpha\right)_\infty}{\left(\frac{1}{x_2^2}; \alpha\right)_\infty} = \frac{\left(\frac{a}{x_2^2}; \alpha\right)_\infty}{\left(\frac{1}{x_2^2}; \alpha\right)_\infty}\frac{1}{\left(\frac{\alpha}{x_2^2}; \alpha\right)_m} \\ \lim_{d\to\infty}\frac{(a^{m+1}; \alpha)_{d-m}}{(\alpha; \alpha)_{d-m}} &= \frac{1}{(\alpha; \alpha)_m}\end{aligned} \tag{D.55}$$

To obtain the expression

$$\begin{aligned}\lim_{d\to\infty}\frac{g(d+1)}{x_2^d} &= \frac{\left(\frac{a}{x_2^2}; \alpha\right)_\infty}{\left(\frac{1}{x_2^2}; \alpha\right)_\infty}\sum_{m=0}^{\infty}\frac{\alpha^{m(m-1)/2}}{\left(\frac{\alpha}{x_2^2}; \alpha\right)_m (\alpha; \alpha)_m}\left(\frac{V}{\cos(K/2)x_2}\right)^m = \\ &= \frac{\left(\frac{a}{x_2^2}; \alpha\right)_\infty}{\left(\frac{1}{x_2^2}; \alpha\right)_\infty} {}_1\phi_1\left(0; \frac{\alpha}{x_2^2}; \alpha, -\frac{V}{\cos(K/2)x_2}\right) .\end{aligned} \tag{D.56}$$

This concludes that the eigenvalues ϵ have to satisfy the equation

$${}_1\phi_1\left(0; \frac{\alpha}{x_2^2(\epsilon)}; \alpha, -\frac{V}{\cos(K/2)x_2(\epsilon)}\right) = 0 . \tag{D.57}$$

In general this equation only has a finite number of solutions, dependent on the interaction strength V, in contrast to the infinitely many bound-states of the discrete one-dimensional hydrogen atom.

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Eigenständigkeitserklärung

Hiermit versichere ich, dass ich die vorliegende Masterarbeit selbstständig verfasst habe. Ich versichere, dass ich keine anderen als die angegebenen Quellen benutzt und alle wörtlich oder sinngemäß aus anderen Werken übernommenen Aussagen als solche gekennzeichnet habe, und dass die eingereichte Arbeit weder vollständig noch in wesentlichen Teilen Gegenstand eines anderen Prüfungsverfahren gewesen ist.

Ort, Datum

Maximilian Bayer

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