A spin chain model with non-Hermitian interaction: the Ising quantum spin chain in an imaginary field

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Abstract

We investigate a lattice version of the Yang–Lee model which is characterized by a non-Hermitian quantum spin chain Hamiltonian. We propose a new way to implement $\mathcal{PT}$-symmetry on the lattice, which serves to guarantee the reality of the spectrum in certain regions of values of the coupling constants. In that region of unbroken $\mathcal{PT}$-symmetry, we construct a Dyson map, a metric operator and find the Hermitian counterpart of the Hamiltonian for small values of the number of sites, both exactly and perturbatively. Besides the standard perturbation theory about the Hermitian part of the Hamiltonian, we also carry out an expansion in the second coupling constant of the model. Our constructions turn out to be unique with the sole assumption that the Dyson map is Hermitian. Finally, we analyse the magnetization of the chain in the z- and x-direction.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

It has been known for about 30 years that ordinary second-order phase transitions can be described by the Yang–Lee model [1–3]. This model admits a quantum field theoretical description in the form of a Landau–Ginzburg Hamiltonian for a scalar field ϕ with an additional ϕ^3-interaction and a term linear in the scalar field with an imaginary coupling constant. The model has been identified [4] as a perturbation of the $\mathcal{M}_{5,2}$-model in the $\mathcal{M}_{p,q}$-series of minimal conformal field theories [5]. It is the simplest non-unitary model in this infinite class of models, which are all characterized by the condition $p - q > 1$ and whose corresponding Hamiltonians are all expected to be non-Hermitian.

Here we shall investigate a discretized lattice version of the Yang–Lee model considered by von Gehlen [6, 7], which is an Ising quantum spin chain in the presence of a magnetic field in the z-direction as well as a longitudinal imaginary field in the x-direction. The corresponding Hamiltonian for a chain of length N is given by

$$H(\lambda, \kappa) = -\frac{1}{2} \sum_{j=1}^{N} \left(\sigma_j^z + \lambda \sigma_j^x \sigma_{j+1}^x + i\kappa \sigma_j^x \right), \qquad \lambda, \kappa \in \mathbb{R}. \tag{1.1}$$

It acts on a Hilbert space of the form $(\mathbb{C}^2)^{\otimes N}$ where we employed the standard notation for the $2^N \times 2^N$-matrices $\sigma_i^{x,y,z} = \mathbb{I} \otimes \mathbb{I} \otimes \cdots \otimes \sigma^{x,y,z} \otimes \cdots \otimes \mathbb{I} \otimes \mathbb{I}$ with Pauli matrices describing spin 1/2 particles

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{1.2}$$

as ith factor acting on the site i of the chain. Their commutation relations are direct sums of su(2) algebras

$$\begin{aligned} \left[\sigma_j^x, \sigma_k^y \right] &= 2i\sigma_j^z \delta_{jk}, & \left[\sigma_j^z, \sigma_k^x \right] &= 2i\sigma_j^y \delta_{jk}, \\ \left[\sigma_j^y, \sigma_k^z \right] &= 2i\sigma_j^x \delta_{jk}, & \text{with} \quad j, k &= 1, \ldots, N. \end{aligned} \tag{1.3}$$

A further real parameter β may be introduced into the model by allowing different types of boundary conditions $\sigma_{N+1}^{x,y,z} = \beta \sigma_1^{x,y,z}$, albeit here we will only consider the case of periodic boundary conditions and take $\beta = 1$.

Since all Pauli matrices are Hermitian, it is obvious that $H(\lambda, \kappa)$ is non-Hermitian:

$$H^\dagger(\lambda, \kappa) = H(\lambda, -\kappa) \neq H(\lambda, \kappa). \tag{1.4}$$

This poses immediately two questions: first, is the spectrum still real, despite the fact that the vital property of Hermiticity which guarantees this is given up and second is it still possible to formulate a meaningful quantum mechanical description associated with this type of Hamiltonians? These issues have attracted a considerable amount of attention in the last 10 years, since the seminal paper by Bender and Boettcher [8] and meanwhile many satisfying answers have been found to most of them; for recent reviews, see [9–11].

Our manuscript is organized as follows. In section 2, we present various alternatives about how $\mathcal{PT}$-symmetry can be implemented for quantum spin chains. In section 3, we establish our notation and recall some of the well-known facts concerning a consistent quantum mechanical framework for $\mathcal{PT}$-symmetric systems. We analyse model (1.1) in sections 4 and 5, where the former is devoted to non-perturbative and the latter to perturbative results. In section 6, we compute the magnetization for model (1.1) and we state our conclusions in section 7.

2. $\mathcal{PT}$-symmetry for spin chains

Preceding the above-mentioned recent activities von Gehlen found numerically [6, 7] that for certain values of the dimensional parameters λ and κ, the eigenvalues for $H(\lambda, \kappa)$ are all real, whereas for the remaining values they occur in complex conjugate pairs. He provided an easy explanation for this feature. Acting adjointly on the Hamiltonian with a spin rotation operator

$$\mathcal{R} = e^{\frac{i\pi}{4} S_z^N} = \prod_{i=1}^{N} \frac{1}{\sqrt{2}} (\mathbb{I} + i\sigma^z)_i, \qquad \text{with} \quad S_z^N = \sum_{i=1}^{N} \sigma_i^z, \quad \mathbb{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{2.1}$$

has the effect of rotating the spins at each site clockwise by $\pi/2$ in the xy-plane, such that the corresponding map acts as $\mathcal{R} : \left(\sigma_i^x, \sigma_i^y, \sigma_i^z\right) \to \left(-\sigma_i^y, \sigma_i^x, \sigma_i^z\right)$. The resulting Hamiltonian is a $2^N \times 2^N$ non-symmetric matrix with real entries given by

$$\hat{H}(\lambda, \kappa) = \mathcal{R}H(\lambda, \kappa)\mathcal{R}^{-1} = -\frac{1}{2}\sum_{i=1}^{N}\left(\sigma_i^z + \lambda\sigma_i^y\sigma_{i+1}^y - \mathrm{i}\kappa\sigma_i^y\right). \tag{2.2}$$

Its eigenvalues and those of $H(\lambda, \kappa)$ are therefore either all real or occur in complex conjugate pairs. This is precisely the well-known behaviour one finds when $H(\lambda, \kappa)$ is symmetric with respect to an anti-linear operator [12–16], which as mentioned above has recently attracted a lot of attention. In quantum mechanical or field theoretical models, the anti-linear operator is commonly taken to be the $\mathcal{PT}$-operator, which carries out a simultaneous parity transformation $\mathcal{P} : x \to -x$ and time reversal $\mathcal{T} : t \to -t$. When acting on complex valued functions, the anti-linear operator $\mathcal{T}$ is understood to act as complex conjugation. Real eigenvalues are then found for unbroken $\mathcal{PT}$-symmetry, meaning that both the Hamiltonian *and* the eigenfunctions remain invariant under $\mathcal{PT}$-symmetry, whereas broken $\mathcal{PT}$-symmetry leads to complex conjugate pairs of eigenvalues.

We will now argue that $\mathcal{PT}$-symmetry on the lattice can be interpreted in various ways. One may for instance reflect the chain across its midpoint via the map $\mathcal{P}' : \sigma_i^{x,y,z} \to \sigma_{N+1-i}^{x,y,z}$ as suggested by Korff and Weston [17] and used thereafter in [18]. It is obvious that the Hamiltonian (1.1) is invariant with regard to this symmetry. However, when keeping the interpretation of $\mathcal{T}$ as a complex conjugation, and thus ensuring that the $\mathcal{P}'\mathcal{T}$-operator is anti-linear, one easily observes that this type of transformation does not leave the Hamiltonian (1.1) invariant, i.e. we have $[\mathcal{P}'\mathcal{T}, H] \neq 0$.

Therefore, we need to implement $\mathcal{PT}$-symmetry in a different way for $H(\lambda, \kappa)$ to be able to analyse its properties along the lines proposed in [12–16]. We propose here that one carries out a parity transformation at each individual site and reflect every spin for instance in the xy-plane on $y = -x$. This is obviously achieved by $\mathcal{R}^2$. As $\mathcal{R}^4 = \prod_{i=1}^{N}(-\mathbb{1})_i = (-1)^N\mathbb{1}^{\otimes N}$ and not the desired identity operator, we take here

$$\mathcal{P} = -\mathrm{i}\mathcal{R}^2 = \mathrm{e}^{\frac{\mathrm{i}\pi}{2}(S^z-\mathbb{1})} = \prod_{i=1}^{N}\sigma_i^z, \qquad \text{with} \quad \mathcal{P}^2 = \mathbb{1}^{\otimes N}, \tag{2.3}$$

as our parity operator. Consequently this transformation acts as

$$\mathcal{P} : \left(\sigma_i^x, \sigma_i^y, \sigma_i^z\right) \to \left(-\sigma_i^x, -\sigma_i^y, \sigma_i^z\right). \tag{2.4}$$

Thus, with $\mathcal{T}$ being the usual complex conjugation, which acts on the Pauli matrices as

$$\mathcal{T} : \left(\sigma_i^x, \sigma_i^y, \sigma_i^z\right) \to \left(\sigma_i^x, -\sigma_i^y, \sigma_i^z\right), \tag{2.5}$$

we have identified an anti-linear operator constituting a symmetry of the Hamiltonian (1.1)

$$[\mathcal{PT}, H] = 0. \tag{2.6}$$

This operator provides more information than the transformation (2.2), because we have now in addition a concrete criterion, which distinguishes the regimes of real and complex eigenvalues. We can precisely separate the two domains $U_{\mathcal{PT}}$ and $U_{b\mathcal{PT}}$ in the parameter space of λ and κ defined by the action on the eigenstates $\Phi(\lambda, \kappa)$ of $H(\lambda, \kappa)$

$$\mathcal{PT}\Phi(\lambda, \kappa) \begin{cases} = \Phi(\lambda, \kappa) & \text{for} \quad (\lambda, \kappa) \in U_{\mathcal{PT}} \\ \neq \Phi(\lambda, \kappa) & \text{for} \quad (\lambda, \kappa) \in U_{b\mathcal{PT}.} \end{cases} \tag{2.7}$$

According to the general reasoning provided in [12–16], simultaneous eigenfunctions of $\mathcal{PT}$ and $H(\lambda, \kappa)$, that is for $(\lambda, \kappa) \in U_{\mathcal{PT}}$, are then associated with real eigenvalues whereas in the

regime of broken $\mathcal{PT}$-symmetry, that is $(\lambda, \kappa) \in U_{b\mathcal{PT}}$, the eigenvalues emerge in complex conjugate pairs.

From the above, it is clear that we may define equally well different types of $\mathcal{PT}$-operators closely related to the one introduced in (2.3). For instance, we can define

$$\mathcal{P}_x := \prod_{i=1}^{N} \sigma_i^x \qquad \text{and} \qquad \mathcal{P}_y := \prod_{i=1}^{N} \sigma_i^y, \qquad (2.8)$$

which obviously act as

$$\mathcal{P}_x : \left(\sigma_i^x, \sigma_i^y, \sigma_i^z\right) \to \left(\sigma_i^x, -\sigma_i^y, -\sigma_i^z\right) \quad \text{and} \quad \mathcal{P}_y : \left(\sigma_i^x, \sigma_i^y, \sigma_i^z\right) \to \left(-\sigma_i^x, \sigma_i^y, -\sigma_i^z\right). \tag{2.9}$$

Clearly these parity operators cannot be used in the same way as $\mathcal{P}$ in (2.3) to introduce a $\mathcal{PT}$-symmetry for $H(\lambda, \kappa)$ when keeping $\mathcal{T}$ unchanged. However, they serve to treat non-Hermitian Hamiltonians of a different kind, such as obvious modifications of $H(\lambda, \kappa)$ and also to allow for alternative treatments of non-Hermitian spin chains, such as the XXZ-spin-chain in a magnetic field [19]:

$$H_{XXZ} = \frac{1}{2} \sum_{i=1}^{N-1} \left[\left(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \Delta_+ \left(\sigma_i^z \sigma_{i+1}^z - 1\right)\right] + \frac{\Delta_-}{2} \left(\sigma_1^z - \sigma_N^z\right), \tag{2.10}$$

with $\Delta_\pm = (q \pm q^{-1})/2$ previously studied in [17, 18]. Obviously when $q \notin \mathbb{R}$ this Hamiltonian is non-Hermitian, but we observe that it is $\mathcal{PT}$-symmetric when using any of the parity operators defined in (2.8) and keeping $\mathcal{T}$ to be the usual complex conjugation

$$[\mathcal{P}_x \mathcal{T}, H_{XXZ}] = 0 \qquad \text{and} \qquad [\mathcal{P}_y \mathcal{T}, H_{XXZ}] = 0. \tag{2.11}$$

Thus, besides reflecting the chain across its midpoint in form of a 'macro-reflections', as suggested in [17], we may also carry out the parity transformations on each individual side. It appears that these 'micro-reflections' (2.3), (2.8) allow for a wider range of possibilities, such as for instance Hamiltonians of the type $H(\lambda, \kappa)$ in (1.1), which could not be tackled with $\mathcal{P}' : \sigma_i^{x,y,z} \to \sigma_{N+1-i}^{x,y,z}$. The different possibilities are simply manifestations of the well-known ambiguities non-Hermitian Hamiltonians possess with regard to their operator content [21]. This also means that the symmetries (2.11) will lead to a different kind of physical systems than those identified in [17].

It is well known that H_{XXZ} can be expressed in terms of generators of a Temperley–Lieb algebra E_i, i.e. simply by writing the Hamiltonian alternatively as $H_{XXZ} = \sum_{i=1}^{N-1} E_i$. It is then trivial to see that the algebra remains invariant under a $\mathcal{PT}$-transformation when realized as (2.8): $\mathcal{T} : E_i \to E_i^*$, $\mathcal{P}_{x,y} : E_i \to E_i^*$, such that $\mathcal{P}_{x,y}\mathcal{T} : E_i \to E_i$. On the other hand when implementing the 'macro-reflection' on the entire chain, the $\mathcal{P}'\mathcal{T}$-symmetry on the generators is broken, i.e. $\mathcal{P}'\mathcal{T} : E_i \to E_{N+1-i}$, as was found in [17].

A further interesting non-Hermitian quantum spin chain has recently been investigated by Deguchi and Ghosh [20]:

$$H_{DG} = \sum_{i=1}^{N} \left(\kappa_{zz} \sigma_i^z \sigma_{i+1}^z + \kappa_x \sigma_i^x + \kappa_y \sigma_i^y\right), \tag{2.12}$$

with $\kappa_{zz} \in \mathbb{R}$ and $\kappa_x, \kappa_y \in \mathbb{C}$. Clearly when κ_x or $\kappa_y \notin \mathbb{R}$, the Hamiltonian H_{DG} is not Hermitian, which is the case we will consider. As the previous model also the quasi-Hermitian transverse Ising model allows for different types of realizations for the $\mathcal{PT}$-symmetry. We easily observe that the macro-reflections cannot be implemented

$$[\mathcal{P}'\mathcal{T}, H] \neq 0, \tag{2.13}$$

whereas all the micro-reflections can be realized

$$
\begin{aligned}
[\mathcal{PT}, H] = 0 \qquad &\text{for} \quad \kappa_x, \kappa_y \in i\mathbb{R}, \\
[\mathcal{P}_{x/y}\mathcal{T}, H] = 0 \qquad &\text{for} \quad \kappa_{x/y} \in \mathbb{R}, \quad \kappa_{y/x} \in i\mathbb{R}.
\end{aligned}
\tag{2.14}
$$

Once again these different possibilities raise the question about the uniqueness of the operator content in the model.

Having an explanation for the nature of the eigenvalue spectra, it is left to show that one may in addition construct a meaningful metric for this Hamiltonian with well-defined quantum mechanical observables associated with it. As already indicated, the metric is not even expected to be unique so that, unlike as for the Hermitian case, the observables are no longer defined by the Hamiltonian alone [21]. It remains therefore ambiguous what Hamiltonians of the type $H(\lambda, \kappa)$ describe in terms of physical observables. Having constructed a metric one may often also compute an isospectral Hermitian counterpart for $H(\lambda, \kappa)$ for which the physical observables have the standard meaning.

One of the main purposes of this manuscript is that of finding the Hermitian counterparts of the Hamiltonian (1.1) and studying in some detail (at least for small N) how many such Hermitian Hamiltonians can be constructed.

3. Generalities

3.1. A new metric and an isospectral Hermitian partner from $\mathcal{PT}$-symmetry

For the sake of self-consistency, we briefly recall the well-known procedure [12–16] of how to construct a meaningful metric and isospectral Hermitian counterpart, h, for a non-Hermitian Hamiltonian, H. We assume the Hamiltonian to be diagonalizable and to possess a discrete spectrum. Being non-Hermitian, the Hamiltonian has non-identical left $|\Phi\rangle$ and right eigenvectors $|\Psi\rangle$ with eigenvalue equations

$$
H|\Phi_n\rangle = \varepsilon_n|\Phi_n\rangle \qquad \text{and} \qquad H^\dagger|\Psi_n\rangle = \epsilon_n|\Psi_n\rangle \qquad \text{for} \quad n \in \mathbb{N}.
\tag{3.1}
$$

The eigenvectors are in general not orthogonal $\langle\Phi_n|\Phi_m\rangle \neq \delta_{nm}$ but form a biorthonormal basis:

$$
\langle\Psi_n|\Phi_m\rangle = \delta_{nm}, \qquad \sum_n |\Phi_n\rangle\langle\Psi_n| = \mathbb{I}.
\tag{3.2}
$$

We assume the existence of a self-adjoint, but not necessarily positive, parity operator $\mathcal{P}$ whose adjoint action conjugates the Hamiltonian

$$
H^\dagger = \mathcal{P}H\mathcal{P} \qquad \text{with} \qquad \mathcal{P}^2 = \mathbb{I}.
\tag{3.3}
$$

The action of this operator on the eigenvectors

$$
\mathcal{P}|\Phi_n\rangle = s_n|\Psi_n\rangle \qquad \text{with} \qquad s_n = \pm 1
\tag{3.4}
$$

defines the signature $s = (s_1, s_2, \ldots, s_n)$, which serves to introduce the so-called $\mathcal{C}$-operator[1]:

$$
\mathcal{C} := \sum_n s_n|\Phi_n\rangle\langle\Psi_n|,
\tag{3.5}
$$

satisfying

$$
[\mathcal{C}, H] = 0, \qquad [\mathcal{C}, \mathcal{PT}] = 0, \qquad \mathcal{C}^2 = \mathbb{I}.
\tag{3.6}
$$

---

[1] This is an unfortunate notation and it should be pointed out that the operator is not related to the standard charge conjugation operator in quantum field theory.

Next we employ this operator to define a new operator ρ, which also relates the Hamiltonian to its conjugate

$$\rho := \mathcal{PC}, \qquad H^\dagger \rho = \rho H. \tag{3.7}$$

Depending now on the assumptions made for ρ, such systems allow for different types of conclusions. When ρ is positive and Hermitian, but not necessarily invertible, the system is referred to as quasi-Hermitian [22, 21]. In this case, the existence of a definite metric is guaranteed and the eigenvalues are real. In turn when ρ is invertible and Hermitian, but not necessarily positive, the system is called pseudo-Hermitian [23–25]. For this type of scenario, the eigenvalues are always real but no definite conclusions can be made with regard to the existence of a definite metric. Here, we will identify operators ρ which are quasi-Hermitian as well as pseudo-Hermitian.

　　Finally, we may factorize ρ into a new operator[2] η and use it to construct an isospectral Hermitian counterpart for H

$$h = \eta H \eta^{-1} = h^\dagger \qquad \Leftrightarrow \qquad H^\dagger = \rho H \rho^{-1} \quad \text{with} \quad \rho = \eta^\dagger \eta. \tag{3.8}$$

In other words, assuming the existence of an inverse for ρ and its factorization in the form of (3.8), one can derive a Hermitian counterpart h for H and vice versa.

3.2. Expectation values of local observables

As discussed above, when dealing with non-Hermitian Hamiltonians, the standard metric is generally indefinite and therefore a new, physically sensible, metric needs to be defined by means of the construction described before. This amounts to introducing a new inner product $\langle\,|\,\rangle_\rho$ which is defined in terms of the standard inner product $\langle\,|\,\rangle$ as

$$\langle\Phi|\Psi\rangle_\rho := \langle\Phi|\rho\Psi\rangle, \tag{3.9}$$

for arbitrary states, $\langle\Phi|$ and $|\Psi\rangle$. Assuming that all local operators $\mathcal{O}$ in the non-Hermitian theory are related to their counterparts o in the Hermitian theory in the same manner as the corresponding Hamiltonians

$$\eta\mathcal{O}\eta^{-1} = o, \tag{3.10}$$

one finds that a generic matrix element of the operator $\mathcal{O}$ has the form,

$$\langle\Phi|\rho\mathcal{O}|\Psi\rangle = \langle\Phi|\eta^\dagger o \eta|\Psi\rangle = \langle\phi|o|\psi\rangle, \tag{3.11}$$

where $|\Psi\rangle$ and $\langle\Phi|$ are eigenstates of the non-Hermitian Hamiltonian and its conjugate, respectively. The states $|\psi\rangle$ and $\langle\phi|$ are related to the previous two states by $|\psi\rangle = \eta|\Psi\rangle$ and $\langle\phi| = \langle\Phi|\eta^\dagger$, that is, they are eigenstates of the Hermitian Hamiltonian corresponding to the same eigenvalues. Equation (3.11) will be used later in this paper for the computation of various kinds of expectation values.

3.3. Perturbation theory

In most cases the above-mentioned operators cannot be computed exactly and one has to resort to a perturbative analysis. Let us recall the main features of such a treatment. To start with it is convenient to separate the Hamiltonian into its Hermitian and non-Hermitian part as $H(\lambda, \kappa) = h_0(\lambda) + i\kappa h_1$, where h_0 and h_1 are both Hermitian with κ being a real coupling

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[2] When η is Hermitian, it just corresponds to a Dyson transformation [26] employed in the so-called Holstein–Primakov method [27]. For practical purposes, it is useful to have a name for this operator and therefore we refer to η from now on as the Dyson map.

constant. The latter term may then be treated as the perturbing term. For our concrete case (1.1), the individual components are

$$h_0(\lambda) = -\frac{1}{2}\sum_{i=1}^{N}\left(\sigma_i^z + \lambda\sigma_i^x\sigma_{i+1}^x\right) \qquad \text{and} \qquad h_1 = -\frac{1}{2}\sum_{i=1}^{N}\sigma_i^x, \qquad (3.12)$$

such that $h_0(\lambda)$ corresponds to the Ising spin chain coupled to a magnetic field in the z-direction and the perturbing term is an imaginary magnetic field in the x-direction. In order to determine η, ρ and h, we can now solve either of the two equations in (3.8). Here we decide to commence with the latter. Making the further assumption that η is Hermitian and of the form $\eta = \mathrm{e}^{q/2}$, this amounts to solving

$$H^\dagger = \mathrm{e}^q\, H\, \mathrm{e}^{-q} = H + [q, H] + \frac{1}{2}[q, [q, H]] + \frac{1}{3!}[q, [q, [q, H]]] + \cdots, \qquad (3.13)$$

where we have employed the Baker–Campbell–Hausdorff identity. Writing H and $H^\dagger$ in terms of h_0 and h_1, equation (3.13) becomes

$$2\mathrm{i}\kappa h_1 + \mathrm{i}\kappa[q, h_1] + \frac{\mathrm{i}\kappa}{2}[q, [q, h_1]] + \cdots = [h_0, q] + \frac{1}{2}[q, [h_0, q]] + \cdots. \qquad (3.14)$$

For most non-Hermitian Hamiltonians, such as for our model (1.1), this equation is very difficult to solve for q. When the $(\ell + 1)$-fold commutator of q with h_0 vanishes, useful closed formulae for h and H were found in [28], see (3.14) and (3.15) therein.

One may also impose some further structure on q and expand it as

$$q = \sum_{k=1}^{\infty}\kappa^{2k-1}q_{2k-1}, \qquad (3.15)$$

so that each perturbative contribution q_{2k-1} is a κ-independent matrix. For models of the form considered here, only odd powers of κ appear in the perturbative expansion. This is essentially due to the fact that H and $H^\dagger$ are related to each other by $\kappa \to -\kappa$. Substituting the expansion (3.15) into equation (3.14), one finds a set of equations for $q_1, q_3, q_5, \ldots$ by equating those terms in (3.14) which are of the same order in perturbation theory in κ. The first few equations are given by

$$[h_0, q_1] = 2\mathrm{i}h_1, \qquad (3.16)$$

$$[h_0, q_3] = \frac{\mathrm{i}}{6}[q_1, [q_1, h_1]], \qquad (3.17)$$

$$[h_0, q_5] = \frac{\mathrm{i}}{6}[q_1, [q_3, h_1]] + \frac{\mathrm{i}}{6}[q_3, [q_1, h_1]] - \frac{\mathrm{i}}{360}[q_1, [q_1, [q_1, h_1]]]. \qquad (3.18)$$

As we can see easily, they can be solved recursively, namely once q_1 is known, one can solve for q_3 and so on. A closed expression for the commutator $[h_0, q_n]$ in terms of commutators $[q_m, h_1]$ with $m < n$ was derived in [18]. Perturbation theory has been carried out in the past for various non-Hermitian models, e.g. [16, 18, 28–31].

The model at hand is special in the sense that it involves two coupling constants, i.e. κ and λ, such that it allows for an alternative perturbative expansion in terms of the latter. Indeed we will demonstrate below that the case $\lambda = 0$ can be solved exactly and we can therefore expand around that solution. Proceeding similarly as for the κ-perturbation theory, we separate the Hamiltonian into its single spin contribution and into the nearest neighbor interaction term $H(\lambda, \kappa) = \tilde{H}_0(\kappa) + \lambda\tilde{h}_1$ with

$$\tilde{H}_0(\kappa) = -\frac{1}{2}\sum_{i=1}^{N}\left(\sigma_i^z + \mathrm{i}\kappa\sigma_i^x\right) \qquad \text{and} \qquad \tilde{h}_1 = -\frac{1}{2}\sum_{i=1}^{N}\sigma_i^x\sigma_{i+1}^x. \qquad (3.19)$$

We stress that the counterparts of (3.16)–(3.18) in the well-known κ-expansion explained above differ substantially in the λ-expansion. The details will be explained in the main part of the manuscript below. Having the option to construct two perturbative series, we in principle have in addition the possibility to combine them in a manner that has proved to be very successful in the context of high-intensity laser physics [32].

3.4. Ambiguities in the physical observables

As mentioned previously, one can argue that the metric ρ is not unique. In the perturbation theory framework, this can be easily seen from the fact that equations (3.16)–(3.18) (and any other equations arising at higher orders in perturbation theory) admit many different solutions. The non-uniqueness of η or, equivalently, the fact that several independent Hermitian Hamiltonians h may exist which are all related to the same non-Hermitian Hamiltonian by different unitary transformations is well known in the literature. Indeed, this fact has been noticed already in the past [21, 30, 33–36] and is currently still an object of debate [37, 38].

Assuming now the Dyson map η in (3.8) to be Hermitian and related to the operators $\mathcal{P}$, $\mathcal{C}$ and ρ as defined in (3.7), we simply obtain

$$\eta = \eta^{\dagger} \quad \Rightarrow \quad \eta^2 = \rho = \mathcal{P}\mathcal{C}. \tag{3.20}$$

Writing $\eta = e^{q/2}$, it is obvious that we can always add to q any matrix b that commutes with the full Hamiltonian $[H, b] = 0$ and with q, $[q, b] = 0$:

$$h = e^{q/2+b} H e^{-q/2-b} = e^{q/2} H e^{-q/2}, \tag{3.21}$$

and still solve equations (3.8). This kind of ambiguity is not very interesting, as it will not change h and therefore not lead to new physics. A somewhat less trivial ambiguity was pointed out in [30], which will generate different types of Hermitian counterparts to H. It originates from the fact that we can always add to $q_1, q_3, q_5, \ldots$ any matrix commuting with h_0 as we may easily observe in equations (3.16)–(3.18). Below we will see that in principle for specific examples, many such matrices can be found.

However, by relating η to the operators $\mathcal{C}$ and $\mathcal{P}$ as in (3.20), we are introducing further constraints on the form of η. These constraints follow from equations (3.6), particularly the last two equations there. Using the explicit form (3.20), they can be rewritten as

$$\mathcal{P}\mathcal{T} e^q \mathcal{P}\mathcal{T} = e^q, \qquad \mathcal{P} e^q \mathcal{P} = e^{-q}. \tag{3.22}$$

by employing the equality $\mathcal{C} = \eta^2 \mathcal{P} = e^q \mathcal{P}$. We assume that $\mathcal{P}$ and $\mathcal{T}$ commute. In order for (3.22) to be satisfied, it is required that

$$\mathcal{P}q\mathcal{P} = \mathcal{T}q\mathcal{T} = -q, \tag{3.23}$$

and consequently

$$\mathcal{P}q_{2k-1}\mathcal{P} = \mathcal{T}q_{2k-1}\mathcal{T} = -q_{2k-1}, \qquad \forall\, k \in \mathbb{Z}^+. \tag{3.24}$$

Below, we will show that these constraints are sufficient in many cases to fix the operator η and therefore the metric completely. However, it should be noted that these arguments are based on the assumption that ρ acquires the form (3.20) and furthermore that the parity operator is unique, which as we exemplified (2.8) is not always the case.

4. The Yang–Lee quantum chain: non-perturbative results

We will now employ the general ideas and definitions introduced in the previous subsection for the quantum spin chain Hamiltonian (1.1). In particular, we will show how to obtain exact solutions for the operators η, ρ and h in the two particular situations: (i) λ or κ are vanishing and N is generic and (ii) λ and κ are arbitrary and N is taken to be small.

For large values of N, it will be convenient to use the following abbreviation:

$$S^N_{a_1 a_2 \ldots a_p} := \sum_{k=1}^{N} \sigma^{a_1}_k \sigma^{a_2}_{k+1} \ldots \sigma^{a_p}_{k+p-1}, \qquad \text{for} \quad a_i = x, y, z, u; \quad i = 1, \ldots, p \leqslant N. \quad (4.1)$$

We denote here $\sigma^u = \mathbb{I}$ to allow for non-local, i.e. not nearest neighbor, interactions. In this notation, the Hamiltonian (1.1) reads

$$H(\lambda, \kappa) = h_0(\lambda) + \mathrm{i}\kappa h_1, \qquad \text{with} \quad h_0(\lambda) = -\tfrac{1}{2}\big(S^N_z + \lambda S^N_{xx}\big), \qquad h_1 = -\tfrac{1}{2} S^N_x. \quad (4.2)$$

In what follows it will also be important to use the adjoint action of $\mathcal{P}$, $\mathcal{T}$ and $\mathcal{PT}$ on the generators $S^N_{a_1 a_2 \ldots a_p}$. It is easy to compute

$$\mathcal{P} S^N_{a_1 a_2 \ldots a_p} \mathcal{P} = (-1)^{n_y + n_x} S^N_{a_1 a_2 \ldots a_p}, \qquad (4.3)$$

$$\mathcal{T} S^N_{a_1 a_2 \ldots a_p} \mathcal{T} = (-1)^{n_y} S^N_{a_1 a_2 \ldots a_p}, \qquad (4.4)$$

$$\mathcal{PT} S^N_{a_1 a_2 \ldots a_p} \mathcal{PT} = (-1)^{n_x} S^N_{a_1 a_2 \ldots a_p}, \qquad (4.5)$$

where n_x, n_y are the numbers of indices a_i equal to x, y, respectively. These identities follow directly from definitions (2.4) and (2.5).

4.1. Limiting cases: $\lambda = 0$ or $\kappa = 0$

Let us start by considering the special case $\lambda = 0$ for which

$$h_0(0) = -\tfrac{1}{2} S^N_z \qquad \text{and} \qquad h_1 = -\tfrac{1}{2} S^N_x. \quad (4.6)$$

Although the Hamiltonian is extremely simple, it is still non-Hermitian, and thus serves as a benchmark to illustrate the above-mentioned notions. For example, a matrix η that relates $H(0, \kappa)$ to its Hermitian counterpart $h(0, \kappa)$ is easily found to be

$$\eta = \mathrm{e}^{q/2} = \mathrm{e}^{-\frac{1}{2}\mathrm{arctanh}(\kappa) S^N_y}. \quad (4.7)$$

Its adjoint action on S^N_x and S^N_z is simply

$$\eta S^N_x \eta^{-1} = \frac{1}{\sqrt{1 - \kappa^2}}\big(\mathrm{i}\kappa S^N_z + S^N_x\big), \qquad \eta S^N_z \eta^{-1} = \frac{1}{\sqrt{1 - \kappa^2}}\big(S^N_z - \mathrm{i}\kappa S^N_x\big), \quad (4.8)$$

which when we evaluate (3.8) yields the Hermitian counterpart to $\tilde{H}_0(\kappa)$ in (3.19)

$$h(0, \kappa) = -\tfrac{1}{2}\sqrt{1 - \kappa^2}\, S^N_z. \quad (4.9)$$

This Hamiltonian describes a spin chain for which no mutual interaction between spins along the chain occurs. An external magnetic field is applied at each site of the chain, whose intensity is governed by the value of κ and is the same at every site. The constraint $-1 < \kappa < 1$ ensures the Hamiltonian $h(0, \kappa)$ and η to be Hermitian. Given the simplicity of $h(0, \kappa)$, we can easily find its full set of eigenstates and eigenvalues, hence those of $H(0, \kappa)$. The operator S^N_z is a diagonal matrix with entries

$$S^N_z = \mathrm{diag}(N, N - 2, \ldots, -N + 2, -N). \quad (4.10)$$

The entries in the diagonal (eigenvalues) are $N - 2p$ with $p = 0, \ldots, N$. They are not necessarily in decreasing order and, except for N and $-N$, all other eigenvalues are degenerate. For example, the eigenvalues $N - 2$ and $2 - N$ are always N times degenerate. This means that there is a single ground state with minimum energy,

$$E_g(\kappa) = -\frac{N}{2}\sqrt{1 - \kappa^2}, \tag{4.11}$$

and the corresponding eigenstate is simply

$$|\psi_g\rangle = \bigotimes_{i=1}^{N} \begin{pmatrix} 1 \\ 0 \end{pmatrix}_i, \tag{4.12}$$

associated with a configuration with all spins 'up', hence aligned with the magnetic field that is being applied at each site of the chain.

The situation when $\kappa = 0$ and λ is arbitrary corresponds to the Hermitian Hamiltonian given by $h_0(\lambda)$, that is the Ising spin chain with a magnetic field in the z-direction. In this case, $\eta = \mathbb{I}$, which is automatically ensured when using perturbation theory. The eigenstates and eigenvalues of this Hamiltonian have been studied in the literature by using the Bethe ansatz approach, see e.g. [39, 40]. In particular, the ground state cannot be written in such a simple form as (4.12), as it will depend on the value of λ. One does know however that, for finite N, it will interpolate between the $\lambda = 0$ case, in which the ground state is (4.12) and the $\lambda \to \infty$ case, in which the ground state will correspond to alternating up–down spins.

Alternatively one may also diagonalize the Hamiltonian by using Jordan–Wigner transformations as for instance in [41].

4.1.1. Uniqueness of the Dyson operator.

In light of the discussion in section 3.4, it is also interesting to investigate the uniqueness of (4.7). Indeed, we will now show that (4.7) is the only solution to (3.8) which is consistent with (3.22) for the Hamiltonian $H(0, \kappa)$. This can be proven in two steps: firstly, we will characterize the subset of matrices and linear combinations thereof that satisfy (3.23) and secondly, we will show that none of these matrices can be in the kernel of $h_0(0)$. Let us define the matrices, which provide a basis for the set of $2^N \otimes 2^N$-Hermitian matrices,

$$M_{a_1 \ldots a_N} = \sigma_1^{a_1} \otimes \cdots \otimes \sigma_N^{a_N}, \qquad \text{with} \qquad a_i = x, y, z \text{ or } u \quad \forall\, i = 1, \ldots, N. \tag{4.13}$$

Recall the definition $\sigma_i^u = \mathbb{I}_i$. Let us consider an arbitrary linear combination of the matrices (4.13). The action of parity and time reversal on such a linear combination is analogous to (4.3) and (4.4). From this it follows that, in order for any linear combination of matrices $M_{a_1, \ldots, a_p}$ to transform as q does in equations (3.23), it must be such that for all matrices in the linear combination n_y is odd and n_x is even (n_x and n_y as defined after equation (4.5)).

We will now argue that no matrix in the kernel of $h_0(0)$ is of this form. There are various ways of having a vanishing commutator $[h_0(0), B] = 0$. The most obvious solution is for B to be a diagonal matrix, as $h_0(0)$ is itself diagonal. In terms of the matrices (4.13), this means selecting out those that are tensor products of σ^z and $\mathbb{I}$ only. There are overall 2^N such matrices and obviously none of them has n_y odd. This would be sufficient to conclude that the solution (4.7) is unique if only the kernel of $h_0(0)$ had dimension 2^N. This is not so because $h_0(0)$ has degenerate eigenvalues.

Any additional matrices in the kernel will be some linear combination of matrices (4.13) involving at least one index x or y. Employing the commutation relations (1.3), it is easy to see that there are basically two kinds of additional matrices that are in the kernel of $h_0(0)$: firstly, the matrices $M_{xyu\ldots u} - M_{yxu\ldots u}$ and generalizations thereof, which are antisymmetric

under the exchange of indices $x \leftrightarrow y$ and violate the condition n_x even and secondly, the matrices $M_{xxu...u} + M_{yyu...u}$ and generalizations thereof, which violate the condition n_y odd and are symmetric under the exchange of indices $x \leftrightarrow y$. Generalizations of these matrices are those obtained by replacing any number of indices u by z and/or permuting indices, as well as other matrices of similar characteristics, such as $M_{xxxxu...u} + M_{yyyyu...u} + M_{xxyyu...u} + M_{yyxxu...u}$ and so on. Since this is more an argument than a proof, we would like to support it with two examples. For $N = 2$,

$$h_0(0) = \text{diag}(-1, 0, 0, 1), \tag{4.14}$$

and the kernel has dimensions 6, as one eigenvalue is twice degenerate. It is generated by the matrices

$$M_{xy} - M_{yx}, \quad M_{xx} + M_{yy}, \quad M_{zz}, \quad M_{zu}, \quad M_{uz} \quad \text{and} \quad M_{uu} = \mathbb{I}. \tag{4.15}$$

For $N = 3$, we have that $h_0(0)$ has four different eigenvalues, two of which are three times degenerate,

$$h_0(0) = \text{diag}\left(-\tfrac{3}{2}, -\tfrac{1}{2}, -\tfrac{1}{2}, \tfrac{1}{2}, -\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}, \tfrac{3}{2}\right). \tag{4.16}$$

The dimension of the kernel then becomes 20. Its generators are the matrices

$$
\begin{aligned}
&M_{xyu} - M_{yxu}, \quad M_{xuy} - M_{yux}, \quad M_{uxy} - M_{uyx}, \\
&M_{xxu} + M_{yyu}, \quad M_{xux} + M_{yuy}, \quad M_{uxx} + M_{uyy}, \\
&M_{xyz} - M_{yxz}, \quad M_{xzy} - M_{yzx}, \quad M_{zxy} - M_{zyx}, \\
&M_{xxz} + M_{yyz}, \quad M_{xzx} + M_{yzy}, \quad M_{zxx} + M_{zyy}, \\
&M_{zzz}, \quad M_{zzu}, \quad M_{zuz}, \quad M_{uzz}, \quad M_{zuu}, \quad M_{uzu}, \quad M_{uuz}, \quad M_{uuu}.
\end{aligned}
\tag{4.17}
$$

As shown before, these examples confirm once more that no element in the kernel of $h_0(0)$ can fulfil the conditions (3.23) and therefore could not be added to q, whilst fulfilling such conditions. Thus no matrices in the kernel of $h_0(0)$ satisfy the conditions (3.23) and the solution (4.7) is unique if the operator $\eta = e^{q/2}$ is to be Hermitian.

4.2. The $N = 2$ case: two sites

We have already identified the $\mathcal{PT}$-symmetry for the Hamiltonian (1.1) with $\mathcal{P}$ given as specified in (2.3) satisfying (3.3). Let us now take the length of the spin chain to be $N = 2$ and compute the quantities as outlined in the previous section.

For two sites, we may chose without loss of generality the boundary conditions to be periodic $\sigma_{N+1}^x = \sigma_1^x$ as any other choice may be achieved simply by a re-definition of λ. In this case, the Hamiltonian (1.1) acquires the simple form of a non-Hermitian 4×4-matrix. In order to make notations clear, we will write this matrix here in the various notations introduced so far,

$$
\begin{aligned}
H(\lambda, \kappa) &= -\frac{1}{2}[\sigma^z \otimes \mathbb{I} + \mathbb{I} \otimes \sigma^z + 2\lambda \sigma^x \otimes \sigma^x + i\kappa(\mathbb{I} \otimes \sigma^x + \sigma^x \otimes \mathbb{I})], \\
&= -\frac{1}{2}[\sigma_1^z + \sigma_2^z + 2\lambda \sigma_1^x \sigma_2^x + i\kappa(\sigma_2^x + \sigma_1^x)], \\
&= -\frac{1}{2}[S_z^2 + \lambda S_{xx}^2 + i\kappa S_z^2] = -
\begin{pmatrix}
1 & \frac{i\kappa}{2} & \frac{i\kappa}{2} & \lambda \\
\frac{i\kappa}{2} & 0 & \lambda & \frac{i\kappa}{2} \\
\frac{i\kappa}{2} & \lambda & 0 & \frac{i\kappa}{2} \\
\lambda & \frac{i\kappa}{2} & \frac{i\kappa}{2} & -1
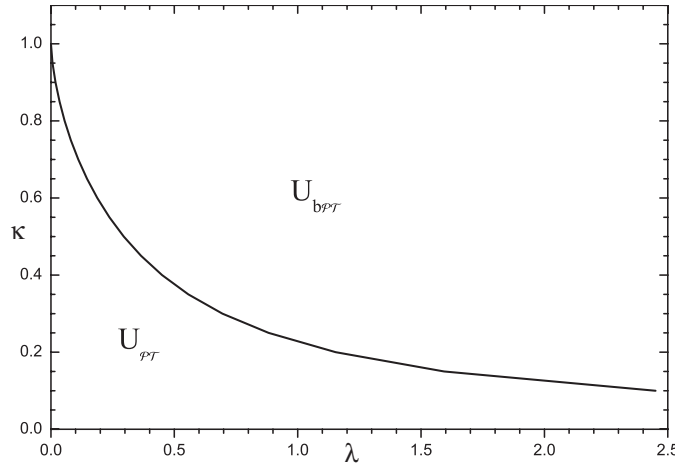\end{pmatrix},
\end{aligned}
\tag{4.18}
$$

Figure 1. Domains of broken and unbroken $\mathcal{PT}$-symmetry for $N = 2$.

where the first line shows the most explicit way of writing the Hamiltonian, the second line shows a simplified version, were the tensor products are omitted and absorbed into the σs as specified after (1.1). The last line uses the notation introduced in (4.1).

At first we shall be concerned with the spectral properties of this Hamiltonian. The two subdomains $U_{\mathcal{PT}}$ and $U_{b\mathcal{PT}}$, as introduced in (2.7), have already been identified numerically in [6] for spin chain lengths up to $N = 19$, that is for matrices up to the remarkable size of $524\,288 \times 524\,288$. For $N = 2$, the eigenvalues for (4.18) are easily computed analytically as the characteristic polynomial factorizes into a third- and first-order polynomial. The discriminant Δ of the third-order polynomial is computed by

$$\Delta = r^2 - q^3 \qquad \text{with} \qquad q = \frac{1}{9}(-3\kappa^2 + 4\lambda^2 + 3), \quad r = \frac{\lambda}{27}(18\kappa^2 + 8\lambda^2 + 9). \quad (4.19)$$

The eigenvalues are guaranteed to be real when the discriminant is smaller or equal to zero, such that $U_{\mathcal{PT}}$ is defined as

$$U_{\mathcal{PT}} = \{\lambda, \kappa : \Delta = \kappa^6 + 8\lambda^2\kappa^4 - 3\kappa^4 + 16\lambda^4\kappa^2 + 20\lambda^2\kappa^2 + 3\kappa^2 - \lambda^2 - 1 \leqslant 0\}. \quad (4.20)$$

The regions $U_{\mathcal{PT}}$ and $U_{b\mathcal{PT}}$ are depicted in figure 1, from which we note that in order to have a real eigenvalue spectrum κ is restricted to take values between 0 and 1, whereas λ is left unbounded $\lambda \in [0, \infty)$.

In [6] the transition line between $U_{\mathcal{PT}}$ and $U_{b\mathcal{PT}}$ was computed numerically for $\lambda = 0.15$ and $\lambda = 1.0$, see table 2 therein. Our analytic expression (4.20) yields for these values the corresponding κ values as $0.644\,960\,193\,843\,4796$ and $0.225\,711\,998\,467\,0051$, respectively. Up to the numerical precision reached in [6], that is ten digits, these values are in precise agreement with the figures reported in [6]. The four real eigenvalues are then computed to

$$\varepsilon_1 = \lambda, \qquad \varepsilon_2 = 2q^{\frac{1}{2}}\cos\left(\frac{\theta}{3}\right) - \frac{\lambda}{3}, \qquad \varepsilon_{3,4} = 2q^{\frac{1}{2}}\cos\left(\frac{\theta}{3} + \pi \mp \frac{2\pi}{3}\right) - \frac{\lambda}{3}, \quad (4.21)$$

where the additional abbreviation $\theta = \arccos(r/q^{3/2})$ has been introduced. We depict these eigenvalues in figure 2, where we observe the typical avoided level-crossing behaviour of the eigenvalues as a function of the parameters [42], i.e. the eigenvalues ε_3 and ε_4 only meet in the exceptional point when they simultaneously become complex.
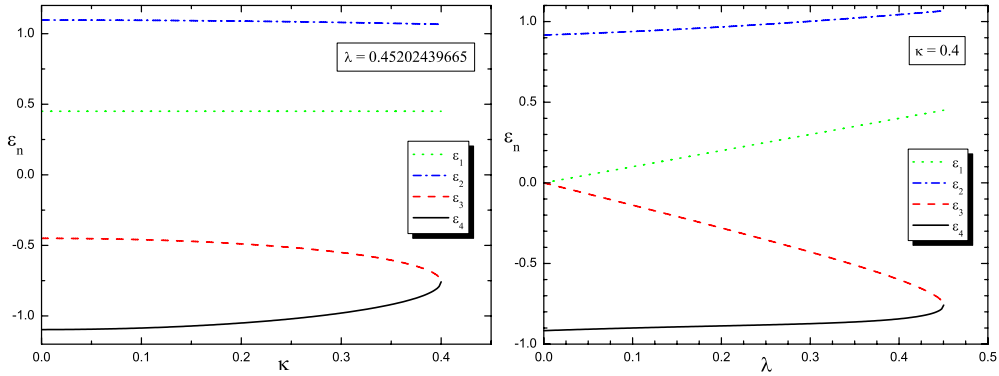
Figure 2. Avoided level crossing: eigenvalues as functions of λ (κ) for fixed κ (λ) for $N = 2$.

For the computations of physical observables, which we will carry out below, it is important to identify the lowest eigenvalue, which turns out to be always ε_4.

Next we compute the right eigenvectors of $H(\lambda, \kappa)$ to

$$|\Phi_1\rangle = (0, -1, -1, 0), \qquad |\Phi_n\rangle = (\gamma_n, -\alpha_n, -\alpha_n, \beta_n), \quad n = 2, 3, 4, \tag{4.22}$$

with $\alpha_n = i\kappa(\lambda - \varepsilon_n + 1)$, $\beta_n = \kappa^2 + 2\lambda^2 + 2\lambda\varepsilon_n$ and $\gamma_n = -\kappa^2 - 2\varepsilon_n^2 + 2\lambda - 2\lambda\varepsilon_n + 2\varepsilon_n$. We verify that left and right eigenvectors are related via a conjugation $|\Psi_n\rangle = \langle\Phi_n|$ and compute the signature as defined in (3.4) to $s = (+, -, +, -)$ for the parity operator (2.3). Normalizing the vectors in (4.22) by dividing with $N_1 = \sqrt{2}$, $N_n = \left(2\alpha_n^2 + \beta_n^2 + \gamma_n^2\right)^{1/2}$ for $n = 2, 3, 4$ we compute the $\mathcal{C}$-operator according to (3.5) to

$$\mathcal{C} = \begin{pmatrix} C_5 & -C_3 & -C_3 & C_4 \\ -C_3 & -C_1 - 1 & -C_1 & C_2 \\ -C_3 & -C_1 & -C_1 - 1 & C_2 \\ C_4 & C_2 & C_2 & 2(C_1 + 1) - C_5 \end{pmatrix}, \tag{4.23}$$

where the matrix entries are

$$\begin{aligned}
C_1 &= \frac{\alpha_4^2}{N_4^2} - \frac{\alpha_2^2}{N_2^2} - \frac{\alpha_3^2}{N_3^2} - \frac{1}{2}, & C_2 &= \frac{\alpha_4\beta_4}{N_4^2} - \frac{\alpha_2\beta_2}{N_2^2} - \frac{\alpha_3\beta_3}{N_3^2}, \\
C_3 &= \frac{\alpha_2\gamma_2}{N_2^2} + \frac{\alpha_3\gamma_3}{N_3^2} - \frac{\alpha_4\gamma_4}{N_4^2}, & C_4 &= \frac{\beta_2\gamma_2}{N_2^2} + \frac{\beta_3\gamma_3}{N_3^2} - \frac{\beta_4\gamma_4}{N_4^2}, \\
C_5 &= \frac{\gamma_2^2}{N_2^2} + \frac{\gamma_3^2}{N_3^2} - \frac{\gamma_4^2}{N_4^2}.
\end{aligned} \tag{4.24}$$

We may now verify that $\mathcal{C}$ indeed satisfied the properties (3.6) upon the use of the identities

$$\begin{aligned}
C_2 &= C_2 C_5 - C_3 C_4, & C_3 &= C_5 C_3 - C_2 C_4 - 2 C_1 C_3, & C_4 &= C_2 C_3 - C_1 C_4, \\
1 &= 2 C_3^2 + C_4^2 + C_5^2, & 0 &= C_2^2 + C_3^2 + 2 C_1 (C_1 + 1).
\end{aligned} \tag{4.25}$$

Next we compute the metric operator in the form $\rho = \mathcal{PC}$ simply from (2.3) and (4.23) to

$$\rho = \begin{pmatrix} C_5 & -C_3 & -C_3 & C_4 \\ C_3 & 1 + C_1 & C_1 & -C_2 \\ C_3 & C_1 & 1 + C_1 & -C_2 \\ C_4 & C_2 & C_2 & 2(1 + C_1) - C_5 \end{pmatrix}. \tag{4.26}$$

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Since $i\alpha_i, \beta_i, \gamma_i \in \mathbb{R}$ it follows that $C_1, iC_2, iC_3, C_4, C_5 \in \mathbb{R}$ and therefore we conclude immediately that ρ is Hermitian. To see whether ρ is also positive, as it ought to be, we compute its eigenvalues

$$y_1 = y_2 = 1 \qquad \text{and} \qquad y_{3/4} = 1 + 2C_1 \pm 2\sqrt{C_1(1 + C_1)}. \qquad (4.27)$$

Since $C_1 > 0$ all eigenvalues of ρ are obviously guaranteed to be positive.

Next we determine the corresponding eigenstates to

$$|r_1\rangle = (0, -1, 1, 0), \quad |r_2\rangle = (C_4, 0, 0, 1 - C_5), \quad |r_{3/4}\rangle = (\tilde{\gamma}_{3/4}, \tilde{\alpha}_{3/4}, \tilde{\alpha}_{3/4}, \tilde{\beta}_{3/4}), \qquad (4.28)$$

with $\tilde{\alpha}_{3/4} = y_{3/4}(C_3 C_4 + C_2(-4C_1 + C_5 - 1))/2 - C_3 C_4$, $\tilde{\beta}_{3/4} = -C_3^2 - C_1 - C_1 C_5 + \left(C_3^2 + C_1(4C_1 - C_5 + 3)\right) y_{3/4}$ and $\tilde{\gamma}_{3/4} = C_1 C_4 - C_2 C_3 + (C_2 C_3 + C_1 C_4) y_{3/4}$. Defining now the matrix $U = \{r_1, r_2, r_3, r_4\}$, whose column vectors are the eigenvectors of ρ, we may take the square root of ρ, such that $\eta = \rho^{1/2} = U D^{1/2} U^{-1}$, where $D = \text{diag}(y_1, y_2, y_3, y_4)$. The isospectral Hermitian counterpart of H results from (3.8) to an XYZ spin chain (with just two sites) in a magnetic field

$$h(\lambda, \kappa) = \eta H \eta^{-1} = U D^{1/2} U^{-1} H U D^{-1/2} U^{-1}. \qquad (4.29)$$

Since we have specified explicitly all matrices on the right-hand side in (4.29), i.e. D, U and H, a simple matrix multiplication yields an analytic expression for $h(\lambda, \kappa)$. We will not report this expression here as it is rather lengthy. Instead we will only evaluate its numerical for two specific choices of λ and κ in order to have benchmarks for the following perturbative calculation

$$h(0.1, 0.5) = \begin{pmatrix} -0.829\,536 & 0 & 0 & -0.060\,6492 \\ 0 & -0.034\,1687 & -0.134\,1687 & 0 \\ 0 & -0.134\,1687 & -0.034\,1687 & 0 \\ -0.060\,6492 & 0 & 0 & 0.897\,873 \end{pmatrix} \qquad (4.30)$$

and

$$h(0.9, 0.1) = \begin{pmatrix} -0.985\,439 & 0 & 0 & -0.890\,532 \\ 0 & -0.009\,4167 & -0.909\,417 & 0 \\ 0 & -0.909\,417 & -0.009\,4167 & 0 \\ -0.890\,532 & 0 & 0 & 1.004\,27 \end{pmatrix}. \qquad (4.31)$$

Note that $h_{23} = h_{32} = h_{22} - \lambda = h_{33} - \lambda$. Alternatively we can bring the isospectral counterpart of $H(\lambda, \kappa)$ into the form

$$h(\lambda, \kappa) = \mu_{xx}^2(\lambda, \kappa) S_{xx}^2 + \mu_{yy}^2(\lambda, \kappa) S_{yy}^2 + \mu_{zz}^2(\lambda, \kappa) S_{zz}^2 + \mu_z^2(\lambda, \kappa) S_z^2. \qquad (4.32)$$

It is clear that the coefficients $\mu_{xx}^2, \mu_{yy}^2, \mu_{zz}^2, \mu_z^2$ can be computed by comparing with (4.29), but once again the expressions are rather lengthy and it is not instructive to report them. They are all real functions of λ and κ. In the next section, we would like to compare this exact result with a perturbative expansion.

We have carried out a similar analysis for the chain with three sites explicitly, albeit the resulting formulae are rather cumbersome to present. In any case for longer chains one has to resort to more sophisticated and less transparent techniques as for instance the Bethe ansatz. Alternatively, we may employ perturbation theory.

5. The Yang–Lee quantum chain: perturbative results

In this section, we want to address the problem of obtaining the matrices η, ρ and h from a perturbative analysis as described in section 3.3. We will study the $N = 2, 3$ and 4 cases in detail and draw some conclusions concerning the analytic expressions of η, ρ and h for generic N.

5.1. The $N = 2$ case: perturbation theory in κ

Despite the fact that $H(\lambda, \kappa)$ is just the 4×4-matrix (4.18), it is actually not easy to find the matrix q in (3.13) exactly. As discussed in section 3.4, it is clear that equations (3.16)–(3.18) as well as the equations that would be obtained for higher orders in perturbation theory admit many solutions. Any solution q_{2k-1} can be modified by adding a matrix that commutes with $h_0(\lambda)$. However, not all solutions obtained in this manner would be valid solutions if equations (3.22) are to hold. For the particular case $N = 2$, we are about to show that these constraints actually select out a unique Hermitian counterpart to the Hamiltonian $H(\lambda, \kappa)$. We will start by finding the most general matrix $q_1(\lambda)$ which solves the identity (3.16). It is quite clear that given one solution $q_1(\lambda)$, any matrix of the form $q_1(\lambda) + B(\lambda)$ with $[h_0(\lambda), B(\lambda)] = 0$ will also be a solution, so we may start by finding all such matrices. In this simple case, there are four basic independent solutions to the equation $[h_0(\lambda), B(\lambda)] = 0$:

$$B_1 = \mathbb{I}, \qquad B_2 = S_{zz}^2, \qquad B_3 = S_{xx}^2 + S_{yy}^2 \qquad \text{and} \qquad B_4 = S_z^2 - \lambda S_{yy}^2. \tag{5.1}$$

Since $h_0(\lambda)$ is a 4×4-diagonalizable matrix, with non-degenerate eigenvalues, there can be at most four independent matrices that commute with it, namely those shown above or combinations thereof. On the other hand, it is clear that any polynomial function of the Hamiltonian $h_0(\lambda)$ would also commute with $h_0(\lambda)$. As the four matrices in (5.1) constitute a basis, we expect to be able to express any power of h_0 as linear combinations of them. Indeed, we find

$$h_0(\lambda)^{2n} = \frac{(1 + \lambda^2)^n}{2} \left(B_1 + \frac{1}{2} B_2 \right) + \frac{\lambda^{2n}}{2} \left(B_1 - \frac{1}{2} B_2 \right), \tag{5.2}$$

$$h_0(\lambda)^{2n+1} = (1 + \lambda^2)^n h_0(\lambda) + \frac{\lambda(1 + \lambda^2)^n - \lambda^{2n+1}}{4} B_3, \tag{5.3}$$

for $n \in \mathbb{N}_0$. Therefore, the most general solution to the first-order equation (3.16) for the present model is

$$q_1(\lambda) = -S_y^2 - \lambda \left(S_{yz}^2 + S_{zy}^2 \right) + \sum_{i=1}^{4} f_i(\lambda) B_i, \tag{5.4}$$

where the $f_i(\lambda)$, $i = 1, 2, 3, 4$, are arbitrary functions of λ.

Before we proceed to determine $q_3(\lambda)$ by solving (3.17) let us comment on the ambiguities and answer the question of whether all solutions (5.4) are compatible with equations (3.22). Specializing equations (4.3) and (4.4) for the matrices in (5.4), we find

$$\mathcal{P} X \mathcal{P} = \mathcal{T} X \mathcal{T} = -X, \qquad \text{for} \quad X = S_y^2, S_{yz}^2, S_{zy}^2, \tag{5.5}$$

whereas

$$\mathcal{P} B_i \mathcal{P} = \mathcal{T} B_i \mathcal{T} = B_i, \qquad \text{for} \quad i = 1, 2, 3, 4. \tag{5.6}$$

These equations imply that the equalities (3.22) can only be satisfied if the functions $f_i(\lambda) = 0$ for $i = 1, 2, 3, 4$. Thus, we have selected out a *unique* solution for $q_1(\lambda)$, namely

$$q_1(\lambda) = -S_y^2 - \lambda \left(S_{yz}^2 + S_{zy}^2 \right). \tag{5.7}$$

More generally, the conditions (3.22) together with the properties (4.3) and (4.4) imply that

- any solutions q_{2k-1} must be linear combinations of matrices (4.1) with n_y odd,
- any solutions q_{2k-1} must be linear combinations of matrices (4.1) with $n_y + n_x$ odd,
- or combining the two conditions above, any solutions q_{2k-1} must be linear combinations of matrices (4.1) with n_y odd and n_x even,

as anticipated in subsection 4.1.1. These conditions then automatically guarantee the validity of the $\mathcal{PT}$-properties (3.24) for the q_{2k-1}. For $N = 2$, this singles out the matrices S_y^2 and $S_{yz}^2 + S_{zy}^2 = 2S_{yz}^2$ in (5.7), so that, even before attempting to solve (3.16), we would already know that it can only be a linear combination of those two matrices. As indicated above, these constraints apply for all other $q_{2k-1}(\lambda)$, with $k > 1$ so that we can safely claim that, at all orders in perturbation theory, the matrices $q_{2k-1}(\lambda)$ must be linear combinations of the form,

$$q_{2k-1}(\lambda) = a_{2k-1}(\lambda)S_y^2 + b_{2k-1}(\lambda)\left(S_{yz}^2 + S_{zy}^2\right), \tag{5.8}$$

where $a_{2k-1}(\lambda)$, $b_{2k-1}(\lambda)$ are real functions of λ. In other words, all the terms in the perturbative expansion of q are linear combinations of the same two matrices. Hence, we can write

$$e^q = e^{\alpha(\lambda,\kappa)S_y^2 + \beta(\lambda,\kappa)(S_{yz}^2 + S_{zy}^2)}, \tag{5.9}$$

which after computing the exponential becomes

$$
\begin{pmatrix}
\frac{\rho(\lambda,\kappa)^2 + \epsilon(\lambda,\kappa)^2 \cosh[2\gamma(\lambda,\kappa)]}{2\gamma(\lambda,\kappa)^2} & -\frac{i\epsilon(\lambda,\kappa)\sinh[2\gamma(\lambda,\kappa)]}{2\gamma(\lambda,\kappa)} & -\frac{i\epsilon(\lambda,\kappa)\sinh[2\gamma(\lambda,\kappa)]}{2\gamma(\lambda,\kappa)} & -\frac{\delta(\lambda,\kappa)\sinh^2[\gamma(\lambda,\kappa)]}{\gamma(\lambda,\kappa)^2} \\
\frac{i\epsilon(\lambda,\kappa)\sinh[2\gamma(\lambda,\kappa)]}{2\gamma(\lambda,\kappa)} & \cosh^2\gamma(\lambda,\kappa) & \sinh^2\gamma(\lambda,\kappa) & -\frac{i\rho(\lambda,\kappa)\sinh[2\gamma(\lambda,\kappa)]}{2\gamma(\lambda,\kappa)} \\
\frac{i\epsilon(\lambda,\kappa)\sinh[2\gamma(\lambda,\kappa)]}{2\gamma(\lambda,\kappa)} & \sinh^2\gamma(\lambda,\kappa) & \cosh^2\gamma(\lambda,\kappa) & -\frac{i\rho(\lambda,\kappa)\sinh[2\gamma(\lambda,\kappa)]}{2\gamma(\lambda,\kappa)} \\
\frac{\delta(\lambda,\kappa)\sinh^2\gamma(\lambda,\kappa)}{\gamma(\lambda,\kappa)^2} & \frac{i\rho(\lambda,\kappa)\sinh[2\gamma(\lambda,\kappa)]}{2\gamma(\lambda,\kappa)} & \frac{i\rho(\lambda,\kappa)\sinh[2\gamma(\lambda,\kappa)]}{2\gamma(\lambda,\kappa)} & \frac{\epsilon(\lambda,\kappa)^2 + \rho(\lambda,\kappa)^2 \cosh[2\gamma(\lambda,\kappa)]}{2\gamma(\lambda,\kappa)^2}
\end{pmatrix},
$$

where

$$\alpha(\lambda,\kappa) = \sum_{k=0}^{\infty} \kappa^{2k+1} a_{2k+1}(\lambda), \qquad \beta(\lambda,\kappa) = \sum_{k=0}^{\infty} \kappa^{2k+1} b_{2k+1}(\lambda) \tag{5.10}$$

and

$$\gamma(\lambda,\kappa) = \sqrt{\alpha(\lambda,\kappa)^2 + 4\beta(\lambda,\kappa)^2}, \qquad \delta(\lambda,\kappa) = \alpha(\lambda,\kappa)^2 - 4\beta(\lambda,\kappa)^2. \tag{5.11}$$

$$\epsilon(\lambda,\kappa) = \alpha(\lambda,\kappa) + 2\beta(\lambda,\kappa), \qquad \rho(\lambda,\kappa) = \alpha(\lambda,\kappa) - 2\beta(\lambda,\kappa). \tag{5.12}$$

Note that, for $\alpha(\lambda,\kappa)$ and $\beta(\lambda,\kappa)$ real, the matrix above is explicitly Hermitian, as it should be. Once the coefficients $\alpha(\lambda,\kappa)$ and $\beta(\lambda,\kappa)$ have been obtained, the Hermitian Hamiltonian (3.8) can be easily computed. The difficulty here is however that general formulae for the coefficients $a_{2k+1}(\lambda)$ and $b_{2k+1}(\lambda)$ are very difficult to obtain. Nonetheless, perturbation theory allows us to compute these coefficients up to very high orders in powers of κ. In order to solve for such high orders, we have resorted to the use of the algebraic manipulation software Mathematica. It allows us to find the entries of the matrix (5.9) as perturbative series in κ and to fix the coefficients $a_{2k+1}(\lambda)$ and $b_{2k+1}(\lambda)$ by matching the entries of $H^\dagger(\lambda,\kappa)$ and $\eta^2 H(\lambda,\kappa)\eta^{-2}$, order by order in perturbation theory, as expected from (3.8). For numerical computations and sufficiently small values of κ this gives results which are very close to the exact values. In tables 1 and 2, we present the coefficients $a_{2k+1}(\lambda)$ and $b_{2k+1}(\lambda)$ up to $k = 7$.

These tables should be understood as follows: in order to obtain the corresponding coefficient the numbers in a given row are to be multiplied by the power of λ (with a minus sign added) at the top of the same column and added up. For example:

$$a_5(\lambda) = -\frac{1}{5} - \frac{244\lambda^2}{15} - \frac{2^8\lambda^4}{5}. \tag{5.13}$$

The only case for which it is easy to conjecture the expressions of $a_{2k+1}(\lambda)$, $b_{2k+1}(\lambda)$ for generic values of k corresponds to $\lambda = 0$. Then $a_{2k+1}(0) = -1/(2k + 1)$ and $b_{2k+1}(0) = 0$, which gives the already known result $\alpha(0,\kappa) = -\text{arctanh}(\kappa)$ and $\beta(0,\kappa) = 0$, see

Table 1. The coefficients $a_{2k+1}(\lambda)$ for $k < 8$.

	$-\lambda^0$	$-\lambda^2$	$-\lambda^4$	$-\lambda^6$	$-\lambda^8$	$-\lambda^{10}$	$-\lambda^{12}$	$-\lambda^{14}$
$a_1(\lambda)$	1	0	0	0	0	0	0	0
$a_3(\lambda)$	$\frac{1}{3}$	$\frac{2^4}{3}$	0	0	0	0	0	0
$a_5(\lambda)$	$\frac{1}{5}$	$\frac{244}{15}$	$\frac{2^8}{5}$	0	0	0	0	0
$a_7(\lambda)$	$\frac{1}{7}$	$\frac{1152}{35}$	$\frac{35\,104}{105}$	$\frac{2^{12}}{7}$	0	0	0	0
$a_9(\lambda)$	$\frac{1}{9}$	$\frac{17\,432}{315}$	$\frac{43\,408}{35}$	$\frac{1890\,368}{315}$	$\frac{2^{16}}{9}$	0	0	0
$a_{11}(\lambda)$	$\frac{1}{11}$	$\frac{289\,616}{3465}$	$\frac{797\,296}{231}$	$\frac{38\,228\,224}{1155}$	$\frac{355\,526\,144}{3465}$	$\frac{2^{20}}{11}$	0	0
$a_{13}(\lambda)$	$\frac{1}{13}$	$\frac{353\,372}{3003}$	$\frac{72\,293\,440}{9009}$	$\frac{655\,729\,408}{5005}$	$\frac{2275\,245\,568}{3003}$	$\frac{15\,442\,769\,920}{9009}$	$\frac{2^{24}}{13}$	0
$a_{15}(\lambda)$	$\frac{1}{15}$	$\frac{7100\,416}{45\,045}$	$\frac{67\,453\,952}{4095}$	$\frac{896\,579\,072}{2145}$	$\frac{58\,903\,814\,656}{15\,015}$	$\frac{717\,363\,822\,592}{45\,045}$	$\frac{12\,73\,503\,367\,168}{45\,045}$	$\frac{2^{28}}{15}$

Table 2. The coefficients $b_{2k+1}(\lambda)$ for $k < 8$.

	$-\lambda$	$-\lambda^3$	$-\lambda^5$	$-\lambda^7$	$-\lambda^9$	$-\lambda^{11}$	$-\lambda^{13}$	$-\lambda^{15}$
$b_1(\lambda)$	1	0	0	0	0	0	0	0
$b_3(\lambda)$	$\frac{4}{3}$	$\frac{2^4}{3}$	0	0	0	0	0	0
$b_5(\lambda)$	$\frac{23}{15}$	$\frac{2^7}{5}$	$\frac{2^8}{5}$	0	0	0	0	0
$b_7(\lambda)$	$\frac{176}{105}$	$\frac{7544}{105}$	$\frac{2^{10}(3)}{7}$	$\frac{2^{12}}{7}$	0	0	0	0
$b_9(\lambda)$	$\frac{563}{315}$	$\frac{49\,136}{105}$	$\frac{212\,816}{105}$	$\frac{2^{16}}{9}$	$\frac{2^{16}}{9}$	0	0	0
$b_{11}(\lambda)$	$\frac{6508}{3465}$	$\frac{335\,576}{1155}$	$\frac{7827\,328}{1155}$	$\frac{164\,005\,504}{3465}$	$\frac{2^{18}(5)}{11}$	$\frac{2^{20}}{11}$	0	0
$b_{13}(\lambda)$	$\frac{88\,069}{45\,045}$	$\frac{4400\,960}{9009}$	$\frac{39\,578\,944}{2145}$	$\frac{1947\,324\,416}{9009}$	$\frac{9037\,578\,752}{9009}$	$\frac{2^{23}(3)}{13}$	$\frac{2^{24}}{13}$	0
$b_{15}(\lambda)$	$\frac{91\,072}{45\,045}$	$\frac{34\,381\,136}{45\,045}$	$\frac{178\,162\,048}{4095}$	$\frac{1068\,366\,848}{1365}$	$\frac{37\,570\,428\,928}{6435}$	$\frac{903\,387\,164\,672}{45\,045}$	$\frac{2^{26}(7)}{15}$	$\frac{2^{28}}{15}$

section 4.1. Having found η, it is straightforward using (3.8) to determine the Hermitian counterpart of $H(\lambda, \kappa)$. In general, we find

$$h(\lambda, \kappa) = e^{q/2} H(\lambda, \kappa) e^{-q/2} = \begin{pmatrix} h_{11}(\lambda, \kappa) & 0 & 0 & h_{14}(\lambda, \kappa) \\ 0 & h_{22}(\lambda, \kappa) & h_{22}(\lambda, \kappa) - \lambda & 0 \\ 0 & h_{22}(\lambda, \kappa) - \lambda & h_{22}(\lambda, \kappa) & 0 \\ h_{14}(\lambda, \kappa) & 0 & 0 & h_{44}(\lambda, \kappa) \end{pmatrix}$$

$$= \frac{h_{22}(\lambda, \kappa) - \lambda + h_{14}(\lambda, \kappa)}{4} S_{xx}^2 + \frac{h_{22}(\lambda, \kappa) - \lambda - h_{14}(\lambda, \kappa)}{4} S_{yy}^2$$

$$+ \frac{h_{11}(\lambda, \kappa) + h_{44}(\lambda, \kappa) - 2h_{22}(\lambda, \kappa)}{8} S_{zz}^2 + \frac{h_{11}(\lambda, \kappa) - h_{44}(\lambda, \kappa)}{4} S_z^2$$

$$+ \frac{h_{11}(\lambda, \kappa) + h_{44}(\lambda, \kappa) + 2h_{22}(\lambda, \kappa)}{4}, \tag{5.14}$$

which is the same kind of structure found in (4.29). The functions $h_{11}(\lambda, \kappa)$, $h_{22}(\lambda, \kappa)$, $h_{14}(\lambda, \kappa)$ and $h_{44}(\lambda, \kappa)$ are real functions of the coupling constants which can be evaluated very accurately for fixed values of λ and κ by using the perturbative results above. In fact, the remaining entries of the matrix are not explicitly zero as functions of $\alpha(\lambda, \kappa)$ and $\beta(\lambda, \kappa)$. They are complicated functions of the latter which when carrying out the perturbation theory result to be zero up order κ^{15}. This is consistent with the exact results obtained before. The

explicit expressions of the entries of $h(\lambda, \kappa)$ in terms of the functions (5.11) and (5.12) are very cumbersome and will therefore not be reported here. Here, we will just present their expression as a series expansion in κ up to order κ^4 (for higher orders, expression become too cumbersome):

$$h_{11}(\lambda, \kappa) = -1 + \left(\frac{1}{2} + \lambda\right)\kappa^2 + \left(\frac{1}{8} + \lambda + \frac{3\lambda^2}{2} + 4\lambda^3\right)\kappa^4 + \mathcal{O}(\kappa^6), \tag{5.15}$$

$$h_{22}(\lambda, \kappa) = -\lambda\kappa^2 - \lambda\left(1 + 4\lambda^2\right)\kappa^4 + \mathcal{O}(\kappa^6), \tag{5.16}$$

$$h_{44}(\lambda, \kappa) = 1 + \left(-\frac{1}{2} + \lambda\right)\kappa^2 + \left(-\frac{1}{8} + \lambda - \frac{3\lambda^2}{2} + 4\lambda^3\right)\kappa^4 + \mathcal{O}(\kappa^6), \tag{5.17}$$

$$h_{14}(\lambda, \kappa) = -\lambda + \lambda\kappa^2 + \left(\frac{3\lambda}{2} + 4\lambda^3\right)\kappa^4 + \mathcal{O}(\kappa^6). \tag{5.18}$$

From this expansion, we can deduce some interesting features which also extend to higher orders in perturbation theory

$$\begin{aligned} h_{11}(-\lambda, \kappa) &= -h_{44}(\lambda, \kappa), & h_{22}(-\lambda, \kappa) &= -h_{22}(\lambda, \kappa), \\ h_{14}(-\lambda, \kappa) &= -h_{14}(\lambda, \kappa). \end{aligned} \tag{5.19}$$

Furthermore, we note that the Hermitian Hamiltonian $h(\lambda, \kappa)$ is an even function of κ, so that the series expansion of its components involves only even powers of the coupling. Finally, as it should be, the Hamiltonian $h(\lambda, \kappa)$ is also $\mathcal{PT}$-symmetric, which follows from the fact that all matrices involved ($S_{xx}^2, S_{yy}^2, S_{zz}^2$ and S_z^2) are invariant under the adjoint action of the operator $\mathcal{PT}$. These are in fact the only matrices that are both $\mathcal{PT}$-symmetric and real. In fact we could have known *a priori* before carrying any computations that $h(\lambda, \kappa)$ has to be some linear combination of $S_{xx}^2, S_{yy}^2, S_{zz}^2$ and S_z^2. Note that the reality of $h(\lambda, \kappa)$ can be expressed by saying that any matrices (4.1) involved must have n_y even, as defined in the paragraph after equation (4.5).

In order to compare with the results obtained in section 4, we give below the numerical values of the entries of the Hermitian Hamiltonian $h(\lambda, \kappa)$ for fixed values of the couplings

$$h_p(0.1, 0.5) = \begin{pmatrix} -0.829\,53\underline{4} & 0 & 0 & -0.060\,6\underline{716} \\ 0 & -0.034\,168\underline{8} & -0.134\,16\underline{9} & 0 \\ 0 & -0.134\,169 & -0.034\,168\underline{8} & 0 \\ -0.060\,6\underline{716} & 0 & 0 & 0.897\,87\underline{2} \end{pmatrix}, \tag{5.20}$$

and

$$h_p(0.9, 0.1) = \begin{pmatrix} -0.985\,439 & 0 & 0 & -0.890\,532 \\ 0 & -0.009\,416\,74 & -0.909\,417 & 0 \\ 0 & -0.909\,417 & -0.009\,416\,74 & 0 \\ -0.890\,532 & 0 & 0 & 1.004\,27 \end{pmatrix}, \tag{5.21}$$

where the subindex p indicates that the Hamiltonians above are approximate, as they have been obtained by using perturbation theory.

We underlined the digits which differ from the exact values computed in (4.30) and (4.31) and note that the perturbative expressions for $h(0.1, 0.5)$ and $h(0.9, 0.1)$ agree extremely well with them, especially for smaller values of κ, as is expected.

In order to see how fast this precision is reached in the perturbation theory, we report in table 3 the relative error for the entry h_{11} order by order up to 15.

Table 3. Relative error = |(perturbative value − exact value)/exact value| for h_{11} in (5.15) order by order in κ-perturbation theory.

$\lambda, \kappa \backslash \mathcal{O}(\kappa)$	2	4	6	8	10	12	14
0.9, 0.1	5.7×10^{-4}	4.6×10^{-5}	4.7×10^{-6}	5.3×10^{-7}	6.4×10^{-8}	8.2×10^{-9}	1.1×10^{-9}
0.1, 0.5	2.5×10^{-2}	6.3×10^{-3}	2.1×10^{-3}	7.5×10^{-4}	2.9×10^{-4}	1.6×10^{-4}	4.7×10^{-5}

We observe that the convergence is fairly fast, which allows us to extract useful information from the perturbation theory even at low order. We shall not be concerned here with more rigorous mathematical arguments regarding the summability and convergence in general.

5.2. The $N = 2$ case: perturbation theory in λ

In the previous section, we have employed the standard version of perturbation theory when dealing with non-Hermitian Hamiltonians of the type (1.1), that is decomposing the Hamiltonian into a Hermitian and a non-Hermitian part as in (3.12) and then treating the non-Hermitian part as the perturbation. Since the Hamiltonian (1.1) depends on two independent coupling constants, κ and λ, it is also natural, albeit less standard, to consider perturbation theory in the coupling constant λ rather than in κ. In other words, we expand around the exact solution for $\lambda = 0$ provided in section 4.1 and treat the nearest neighbour interaction term as perturbation. As announced already in section 3.2., we decompose $H(\lambda, \kappa)$ into

$$H(\lambda, \kappa) = \tilde{H}_0(\kappa) + \lambda \tilde{h}_1, \qquad \text{where} \quad \tilde{H}_0(\kappa) = -\tfrac{1}{2}\big(S_z^N + i\kappa S_x^N\big), \quad \tilde{h}_1 = -\tfrac{1}{2}S_{xx}^N. \quad (5.22)$$

We wish now once again to solve equations (3.8) for the Dyson map η, that is

$$H^\dagger(\lambda, \kappa) = e^w H(\lambda, \kappa) e^{-w}, \qquad (5.23)$$

where we have assumed that η admits the exponential form

$$\eta = e^{w/2} \qquad \text{with} \quad w = \sum_{a=0}^{\infty} \lambda^a w_a(\kappa). \qquad (5.24)$$

At order λ^0, equation (5.23) becomes simply

$$\tilde{H}_0^\dagger(\kappa) = e^{w_0(\kappa)} \tilde{H}_0(\kappa) e^{-w_0(\kappa)}. \qquad (5.25)$$

The solution to this equation for all N was found in subsection 4.1 and corresponds to the Dyson map identified in equation (4.7). For $N = 2$, this means that

$$w_0(\kappa) = -\operatorname{arctanh}(\kappa) S_y^2. \qquad (5.26)$$

Employing once again the Baker–Campbell–Hausdorff identity to select $\mathcal{O}(\lambda)$ terms in (5.23), we find the condition

$$\tilde{h}_1 = e^{w_0(\kappa)} \tilde{h}_1\, e^{-w_0(\kappa)} + \sum_{k=1}^{\infty} \sum_{i=1}^{k} \sum_{\substack{a_i=1, \\ a_{j\neq i}=0}} \frac{1}{k!} [w_{a_1}(\kappa), [w_{a_2}(\kappa), \ldots, [w_{a_k}(\kappa), H_0(\kappa)]\cdots]]. \quad (5.27)$$

Note that, because of the presence of the zeroth order term $w_0(\kappa)$, equation (5.27) involves a sum of infinitely many contributions, as would equations corresponding to higher orders in perturbation theory. Because of this, it would in general be difficult to solve (5.23) using perturbation theory in λ. However, for $N = 2$, we can solve up to high orders in λ by

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exploiting the fact that η must have the structure identified in the previous section. This means that η is a matrix of the form (5.9) with

$$\alpha(\lambda, \kappa) = \sum_{a=0}^{\infty} \lambda^a y_a(\kappa), \qquad \beta(\lambda, \kappa) = \sum_{a=0}^{\infty} \lambda^a z_a(\kappa). \tag{5.28}$$

It is then possible to find the real functions $y_a(\kappa)$ and $z_a(\kappa)$ which solve equation (5.23) order by order in λ by employing Mathematica, as explained in the previous subsection. In this way, we have obtained the functions $y_a(\kappa)$ and $z_a(\kappa)$ above up to order λ^{15}. Here we will just report the first five orders,

$$y_0(\kappa) = -\text{arctanh}(\kappa), \tag{5.29}$$

$$z_1(\kappa) = \frac{y_0(\kappa)}{1 - \kappa^2}, \tag{5.30}$$

$$y_2(\kappa) = -\frac{2(\kappa + 2\kappa^3 + (1 - \kappa^2) y_0(\kappa))}{(1 - \kappa^2)^3}, \tag{5.31}$$

$$z_3(\kappa) = -\frac{2(\kappa + 2\kappa^3 + (1 - \kappa^2 - 2\kappa^4) y_0(\kappa))}{(1 - \kappa^2)^4}, \tag{5.32}$$

$$y_4(\kappa) = \frac{2(\kappa(3 - 5\kappa^2 - 32\kappa^4 - 8\kappa^6) + (3 - 6\kappa^2 - 5\kappa^4 + 8\kappa^6) y_0(\kappa))}{(1 - \kappa^2)^6}, \tag{5.33}$$

$$z_5(\kappa) = \frac{2(\kappa(3 - 5\kappa^2 - 36\kappa^4 - 16\kappa^6) + (3 - 6\kappa^2 - 9\kappa^4 + 28\kappa^6 + 8\kappa^8) y_0(\kappa))}{(1 - \kappa^2)^7}, \tag{5.34}$$

and $y_{2a+1}(\kappa) = z_{2a}(\kappa) = 0$ for all $a = 0, 1, \dots$. From these formulae, it is possible to find an expression for the Hermitian Hamiltonian $h(\lambda, \kappa)$ as a perturbative series in λ. As it should be, one finds the same structure (5.14) with

$$h_{11}(\lambda, \kappa) = -\sqrt{1 - \kappa^2} + \frac{\kappa^2 \lambda}{1 - \kappa^2} - \frac{6(-2 + \kappa^2 + 2\sqrt{1 - \kappa^2})\lambda^2}{(1 - \kappa^2)^{\frac{5}{2}}} + \frac{4\kappa^4 \lambda^3}{(1 - \kappa^2)^4}$$
$$- \frac{2(40 - 44\kappa^2 - 57\kappa^4 + 28\kappa^6 + 8\sqrt{1 - \kappa^2}(-5 + 3\kappa^2 + 8\kappa^4))\lambda^4}{(1 - \kappa^2)^{\frac{11}{2}}} + \mathcal{O}(\lambda^5), \tag{5.35}$$

$$h_{22}(\lambda, \kappa) = -\frac{\kappa^2 \lambda}{1 - \kappa^2} - \frac{4\kappa^4 \lambda^3}{(1 - \kappa^2)^4} + \mathcal{O}(\lambda^5), \tag{5.36}$$

$$h_{44}(\lambda, \kappa) = \sqrt{1 - \kappa^2} + \frac{\kappa^2 \lambda}{1 - \kappa^2} + \frac{6(-2 + \kappa^2 + 2\sqrt{1 - \kappa^2})\lambda^2}{(1 - \kappa^2)^{\frac{5}{2}}} + \frac{4\kappa^4 \lambda^3}{(1 - \kappa^2)^4}$$
$$+ \frac{2(40 - 44\kappa^2 - 57\kappa^4 + 28\kappa^6 + 8\sqrt{1 - \kappa^2}(-5 + 3\kappa^2 + 8\kappa^4))\lambda^4}{(1 - \kappa^2)^{\frac{11}{2}}} + \mathcal{O}(\lambda^5), \tag{5.37}$$

Table 4. Relative error $= |(\text{perturbative value} - \text{exact value})/\text{exact value}|$ for h_{11} in (5.35) order by order in λ-perturbation theory.

$\lambda, \kappa \backslash \mathcal{O}(\lambda)$	2	4	6	8	10	12	14
0.9, 0.1	3.4×10^{-3}	2.3×10^{-5}	1.9×10^{-6}	1.8×10^{-7}	1.9×10^{-8}	2.0×10^{-9}	2.2×10^{-10}
0.1, 0.5	1.1×10^{-3}	6.3×10^{-5}	4.9×10^{-6}	3.6×10^{-7}	3.1×10^{-8}	2.8×10^{-9}	2.6×10^{-10}

$$h_{14}(\lambda, \kappa) = \frac{(-4 + 4\kappa^2 + 3\sqrt{1 - \kappa^2})\lambda}{(1 - \kappa^2)^{\frac{3}{2}}}$$

$$+ \frac{4(8 - 10\kappa^2 - 2\kappa^4 + 4\kappa^6 + \sqrt{1 - \kappa^2}(2 + \kappa^2)(-4 + 5\kappa^2))\lambda^3}{(1 - \kappa^2)^{\frac{9}{2}}} + \mathcal{O}(\lambda^5). \quad (5.38)$$

Note that the same symmetries (5.19) are also found here. We also see once again that $h(\lambda, \kappa)$ is an even function of κ, as only even powers are involved. Computing again numerical values for $h(0.1, 0.5)$ and $h(0.9, 0.1)$, we find almost perfect agreement with the exact results. There is extremely good agreement both with the exact results (4.30) and (4.31) and with the result from perturbation theory in κ (5.20) and (5.21). In order to see how fast this precision is reached in the perturbation theory, we report in table 4 the relative error for the entry h_{11} order by order up to 15. We do so in order to shorten table 4 and at the same time make the comparison between tables 3 and 4 easier. As we can see, convergence is excellent in both cases.

We note that the perturbation theory converges extremely fast, even for large values of λ, for which one would not expect such a behaviour. This can be explained as follows. In the domain of unbroken $\mathcal{PT}$-symmetry, $U_{\mathcal{PT}}$ the allowed values for κ become very small as λ increases. As we note from expressions (5.35)–(5.38) the order of κ increases with the order of λ term by term.

5.3. The $N = 3$ case

We will now carry out an analogous perturbative study in κ for the three sites case. We keep the choice of periodic boundary condition, even though for sites more than two this means some loss of generality. Proceeding as before, we will try to obtain the matrix q perturbatively, by solving the consistency conditions (3.16)–(3.18). Now we have to solve the problem for 8×8 matrices. We commence by computing the kernel of h_0

$$B_1 = \mathbb{I}, \quad B_2 = S_{zz}^3 - \lambda S_{yyz}^3, \quad B_3 = \lambda S_{yy}^3 - (1 - \lambda^2)S_{yyz}^3 - S_{xxz}^3, \quad B_4 = S_{xy}^3 - S_{yx}^3,$$
$$B_5 = S_{zzz}^3, \quad B_6 = S_{xyz}^3 - S_{yxz}^3, \quad B_7 = \lambda S_{xx}^3 + S_z^3 = -2h_0(\lambda),$$
$$B_8 = S_{xx}^3 + S_{yy}^3 + \lambda S_{yyz}^3,$$

in addition to this eight matrices, there are another four, due to the fact that two of the eigenvalues of $h_0(\lambda)$ are degenerate. Hence, the dimension of the kernel is 12,

$$B_9 = S_z^3 - \lambda\left(S_{yy}^3 + S_{zz}^3 - \sigma_1^y\sigma_3^y - \sigma_1^z\sigma_3^z - \sigma_1^x\sigma_3^x\right), \quad B_{10} = \sigma_2^y\sigma_3^y + \sigma_2^z\sigma_3^z + \sigma_2^x\sigma_3^x,$$
$$B_{11} = S_{zz}^3 + \lambda S_{xxz}^3 - \lambda\left(\sigma_1^z + \sigma_3^z + \sigma_1^x\sigma_2^z\sigma_3^x + \sigma_1^y\sigma_2^z\sigma_3^y\right), \quad B_{12} = \sigma_3^z - \sigma_1^x\sigma_2^x\sigma_3^z - \sigma_1^y\sigma_2^y\sigma_3^z,$$
$$(5.39)$$

with $[B_i, h_0(\lambda)] = 0$ for $i = 1, \ldots, 12$. Similarly as in the case $N = 2$, we find

$$\mathcal{P}B_i\mathcal{P} = B_i, \qquad \forall \quad i = 1, \ldots, 12, \quad (5.40)$$

Table 5. The coefficients $\hat{a}_{2k+1}(\lambda)$ and $\hat{d}_{2k+1}(\lambda)$ for $k < 4$.

	$-\lambda^0$	$-\lambda^2$	$-\lambda^4$	$-\lambda^6$	$-\lambda^8$	$-\lambda^{10}$	$-\lambda^{12}$
$\hat{a}_1(\lambda)$	1	0	0	0	0	0	0
$\hat{a}_3(\lambda)$	$\frac{1}{3}$	$\frac{8}{3}$	16	0	0	0	0
$\hat{a}_5(\lambda)$	$\frac{1}{5}$	$\frac{122}{15}$	144	$\frac{5024}{15}$	$\frac{3072}{5}$	0	0
$\hat{a}_7(\lambda)$	$\frac{1}{7}$	$\frac{576}{35}$	$\frac{9616}{15}$	$\frac{432\,832}{105}$	$\frac{1755\,136}{105}$	$\frac{2720\,768}{105}$	$\frac{196\,608}{7}$
$\hat{d}_1(\lambda)$	0	0	0	0	0	0	0
$\hat{d}_3(\lambda)$	0	0	$\frac{2^4}{3}$	0	0	0	0
$\hat{d}_5(\lambda)$	0	$\frac{2}{3}$	$\frac{496}{15}$	$\frac{1184}{15}$	$\frac{2^{10}}{5}$	0	0
$\hat{d}_7(\lambda)$	0	$\frac{2^5}{15}$	$\frac{4432}{35}$	$\frac{86\,848}{105}$	$\frac{65\,024}{15}$	$\frac{754\,688}{105}$	$\frac{2^{16}}{7}$

Table 6. The coefficients $\hat{b}_{2k+1}(\lambda)$ for $k < 4$.

	$-\lambda$	$-\lambda^3$	$-\lambda^5$	$-\lambda^7$	$-\lambda^9$	$-\lambda^{11}$	$-\lambda^{13}$
$\hat{b}_1(\lambda)$	1	0	0	0	0	0	0,
$\hat{b}_3(\lambda)$	$\frac{4}{3}$	$\frac{28}{3}$	$\frac{2^6}{3}$	0	0	0	0
$\hat{b}_5(\lambda)$	$\frac{23}{15}$	$\frac{664}{15}$	$\frac{1568}{5}$	$\frac{3328}{5}$	$\frac{2^{12}}{5}$	0	0,
$\hat{b}_7(\lambda)$	$\frac{176}{105}$	$\frac{4344}{35}$	$\frac{13\,536}{7}$	$\frac{52\,416}{5}$	$\frac{1104\,384}{35}$	$\frac{311\,296}{7}$	$\frac{2^{18}}{7}$

which from equations (3.24) means that no linear combination of the matrices B_i can be added to q_{2k-1} that would be compatible with the constraints (3.22). Therefore, with such constraints, there is a unique solution to (3.16) which has the form,

$$q_1(\lambda) = -S_y^3 - \lambda\left(S_{yz}^3 + S_{zy}^3\right) + 2\lambda^2\left(S_{yyy}^3 - S_{zzy}^3\right). \tag{5.41}$$

As we can see, the two first terms in $q_1(\lambda)$ are a direct generalization of the result for two sites, which hints at the existence of a general pattern. As for the $N = 2$, case we find once again that even before attempting to solve (3.16), we could have predicted from (3.24) that the matrices $q_{2k-1}(\lambda)$ can only be linear combinations of S_y^3, S_{yz}^3, S_{zy}^3, S_{yyy}^3, S_{zzy}^3 and S_{xxy}^3 (for $k = 1$, equation (5.1) tells us though that the coefficient of S_{xxy}^3 is zero. This will change for higher orders in perturbation theory). We can therefore write,

$$q = \hat{\alpha}(\lambda, \kappa)S_y^3 + \hat{\beta}(\lambda, \kappa)\left(S_{yz}^3 + S_{zy}^3\right) + \hat{\gamma}(\lambda, \kappa)S_{yyy}^3 + \hat{\delta}(\lambda, \kappa)S_{xxy}^3 + \hat{\epsilon}(\lambda, \kappa)S_{zzy}^3, \tag{5.42}$$

where

$$\hat{\alpha}(\lambda, \kappa) = \sum_{k=1}^{\infty} \hat{a}_{2k-1}(\lambda)\kappa^{2k-1}, \qquad \hat{\beta}(\lambda, \kappa) = \sum_{k=1}^{\infty} \hat{b}_{2k-1}(\lambda)\kappa^{2k-1}, \tag{5.43}$$

$$\hat{\gamma}(\lambda, \kappa) = \sum_{k=1}^{\infty} \hat{s}_{2k-1}(\lambda)\kappa^{2k-1}, \qquad \hat{\delta}(\lambda, \kappa) = \sum_{k=1}^{\infty} \hat{d}_{2k-1}(\lambda)\kappa^{2k-1}, \tag{5.44}$$

$$\hat{\epsilon}(\lambda, \kappa) = \sum_{k=1}^{\infty} \hat{e}_{2k-1}(\lambda)\kappa^{2k-1}. \tag{5.45}$$

Computing coefficients up to order κ^7 we find the results in tables 5–7.

It is now possible to use these perturbative results to compute $h(\lambda, \kappa)$ for particular values of λ and κ. We find that the structure of the Hermitian counterpart of the original

Table 7. The coefficients $\hat{s}_{2k+1}(\lambda)$ and $\hat{e}_{2k+1}(\lambda)$ for $k < 4$.

	$-\lambda^2$	$-\lambda^4$	$-\lambda^6$	$-\lambda^8$	$-\lambda^{10}$	$-\lambda^{12}$	$-\lambda^{14}$
$\hat{s}_1(\lambda)$	-2	0	0	0	0	0	0
$\hat{s}_3(\lambda)$	-4	-8	$-\frac{2^7}{3}$	0	0	0	0
$\hat{s}_5(\lambda)$	$-\frac{28}{5}$	$-\frac{112}{5}$	$-\frac{2592}{5}$	$-\frac{4608}{5}$	$-\frac{2^{13}}{5}$	0	0
$\hat{s}_7(\lambda)$	$-\frac{232}{35}$	$\frac{288}{35}$	$-\frac{91\,008}{35}$	$-\frac{452\,224}{35}$	$-\frac{356\,352}{7}$	$-\frac{491\,520}{7}$	$\frac{2^{19}}{7}$
$\hat{e}_1(\lambda)$	2	0	0	0	0	0	0
$\hat{e}_3(\lambda)$	$\frac{20}{3}$	$\frac{56}{3}$	$\frac{2^7}{3}$	0	0	0	0
$\hat{e}_5(\lambda)$	$\frac{196}{15}$	$\frac{400}{3}$	$\frac{3872}{5}$	$\frac{6656}{5}$	$\frac{2^{13}}{5}$	0	0
$\hat{e}_7(\lambda)$	$\frac{440}{21}$	$\frac{53\,152}{105}$	$\frac{206\,336}{35}$	$\frac{75\,904}{3}$	$69\,632$	$\frac{622\,592}{7}$	$\frac{2^{19}}{7}$

Hamiltonian is

$$h(\lambda, \kappa) = \mu_{xx}^3(\lambda, \kappa)S_{xx}^3 + \mu_{yy}^3(\lambda, \kappa)S_{yy}^3 + \mu_{zz}^3(\lambda, \kappa)S_{zz}^3 + \mu_z^3(\lambda, \kappa)S_z^3$$
$$+ \mu_{xxz}^3(\lambda, \kappa)S_{xxz}^3 + \mu_{yyz}^3(\lambda, \kappa)S_{yyz}^3 + \mu_{zzz}^3(\lambda, \kappa)S_{zzz}^3, \tag{5.46}$$

which resembles the result for two sites, but includes few extra terms that couple all three sites. The functions $\mu_{xx}^3, \ldots, \mu_{zzz}^3$ are all real functions of the couplings. As for $N = 2$, the Hamiltonian above is $\mathcal{PT}$-symmetric, which follows from the fact that all matrices involved are invariant under the adjoint action of the operator $\mathcal{PT}$ (see equation (4.5)). As for $N = 2$ also, these are the only matrices that are both $\mathcal{PT}$ symmetric and real (notice that, from the definition (4.1) for $N = 3$, it holds that $S_{xxz}^3 = S_{zxx}^3 = S_{xzx}^3$ and $S_{yyz}^3 = S_{zyy}^3 = S_{yzy}^3$).

5.4. The $N = 4$ case

It is interesting to investigate how the perturbative results generalize as we increase the number of sites. The $N = 4$ case is especially interesting as it is the simplest example for which we may see non-local interaction terms in the Hermitian Hamiltonian. There is again only one solution for $q_1(\lambda)$ which is compatible with the conditions (3.24), that is

$$q_1(\lambda) = -S_y^4 - \lambda\big(S_{yz}^4 + S_{zy}^4\big) - \frac{6\lambda^3\big(S_{yuz}^4 - S_{yz}^4 - S_{zy}^4\big)}{40\lambda^2 - 9}$$
$$+ \frac{1}{40\lambda^2 - 9}\big[(9 - 32\lambda^2)\lambda^2\big(S_{yzz}^4 + S_{zzy}^4\big) - 32\lambda^4 S_{zyz}^4 - 2\lambda^2(3 - 16\lambda^2)S_{yyy}^4$$
$$- 3\lambda^2\big(S_{xxy}^4 - 2S_{xyx}^4 + S_{yxx}^4\big) + 2\lambda^3\big(S_{xxyz}^4 - 5S_{xyxz}^4 + S_{xxzy}^4\big)$$
$$+ 2\lambda^3\big(9S_{yzzz}^4 - 7S_{yyyz}^4\big) + 64\lambda^5\big(S_{yyyz}^4 - S_{zzzy}^4\big)\big]. \tag{5.47}$$

In many ways, this is a simple generalization of the results of two and three sites. The matrices that enter the expression are to a large extent the same we find for less sites, but we have now extra contributions involving Pauli matrices sitting at all four sites of the chain, which was to be expected. There are however two major changes

- the dependence on λ of the coefficients is not polynomial anymore,
- the first occurrence of non-local interactions appears through the matrix S_{yuz}^4.

As for lower values of N, it is not difficult to argue that the matrices (4.1) entering the linear combination (5.47) are the only ones that are compatible with (3.22). Hence, as expected, the same structure extends to higher orders in perturbation theory, although expressions become

extremely involved. The table below gives $q_3(\lambda)$ as a sum of terms given by the matrices on the first column multiplied by the corresponding coefficients in the second column,

$q_3(\lambda)$	Coefficients
S_y^4	$\dfrac{-81+72\lambda^2+1892\lambda^4-4224\lambda^6+28\,672\lambda^8-131\,072\lambda^{10}}{3\left(-9+40\lambda^2\right)^2}$
$S_{yz}^4 + S_{zy}^4$	$\dfrac{2916\lambda-22\,842\lambda^3+27\,216\lambda^5+81\,152\lambda^7+251\,904\lambda^9+786\,432\lambda^{11}-6291\,456\lambda^{13}}{3\left(-9+40\lambda^2\right)^3}$
S_{yuz}^4	$-\dfrac{64\lambda^5\left(351+276\lambda^2-8352\lambda^4-4096\lambda^6+65\,536\lambda^8\right)}{3\left(-9+40\lambda^2\right)^3}$
$S_{yzz}^4 + S_{zzy}^4$	$-\dfrac{4\lambda^2\left(-1215+7722\lambda^2+12\,432\lambda^4-151\,808\lambda^6+131\,072\lambda^8-262\,144\lambda^{10}+2097\,152\lambda^{12}\right)}{3\left(-9+40\lambda^2\right)^3}$
S_{zyz}^4	$\dfrac{4\lambda^2\left(1215-16\,065\lambda^2+26\,952\lambda^4+72\,448\lambda^6-2097\,152\lambda^{12}\right)}{3\left(-9+40\lambda^2\right)^3}$
S_{yyy}^4	$\dfrac{4\lambda^2\left(-729+8667\lambda^2-14\,040\lambda^4-97\,024\lambda^6+393\,216\lambda^8-1048\,576\lambda^{10}+2097\,152\lambda^{12}\right)}{3\left(-9+40\lambda^2\right)^3}$
$S_{xxy}^4 + S_{yxx}^4$	$-\dfrac{8\lambda^2\left(243-2079\lambda^2+7752\lambda^4+16\,768\lambda^6-159\,744\lambda^8+262\,144\lambda^{10}\right)}{3\left(-9+40\lambda^2\right)^3}$
S_{xyx}^4	$-\dfrac{4\lambda^2\left(-972+6939\lambda^2-31\,512\lambda^4+82\,176\lambda^6-188\,416\lambda^8+262\,144\lambda^{10}\right)}{3\left(-9+40\lambda^2\right)^3}$
$S_{xxyz}^4 + S_{xxzy}^4$	$-\dfrac{2\lambda^3\left(405-19\,368\lambda^2+146\,048\lambda^4-349\,184\lambda^6-131\,072\lambda^8+1048\,576\lambda^{10}\right)}{3\left(-9+40\lambda^2\right)^3}$
S_{xyxz}^4	$-\dfrac{64\lambda^3\left(81-99\lambda^2-692\lambda^4+672\lambda^6+4096\lambda^8\right)}{3\left(-9+40\lambda^2\right)^3}$
S_{zyyy}^4	$\dfrac{32\lambda^3\left(-567+6390\lambda^2-21\,448\lambda^4+12\,096\lambda^6+49\,152\lambda^8-196\,608\lambda^{10}+524\,288\lambda^{12}\right)}{3\left(-9+40\lambda^2\right)^3}$
S_{yzzz}^4	$-\dfrac{32\lambda^3\left(-729+7290\lambda^2-19\,512\lambda^4-5952\lambda^6+32\,768\lambda^8-65\,536\lambda^{10}+524\,288\lambda^{12}\right)}{3\left(-9+40\lambda^2\right)^3}$

In general we have,

$$
\begin{aligned}
q = {} & \zeta(\lambda,\kappa)S_y^4 + \theta(\lambda,\kappa)\left(S_{zy}^4 + S_{yz}^4\right) + \vartheta(\lambda,\kappa)S_{yuz}^4 \\
& + \mu(\lambda,\kappa)\left(S_{yzz}^4 + S_{zzy}^4\right) + \nu(\lambda,\kappa)S_{zyz}^4 + \xi(\lambda,\kappa)S_{yyy}^4 + \varpi(\lambda,\kappa)\left(S_{xxy}^4 + S_{yxx}^4\right) \\
& + \varrho(\lambda,\kappa)S_{xyx}^4 + \varsigma(\lambda,\kappa)\left(S_{xxyz}^4 + S_{xxzy}^4\right) + \tau(\lambda,\kappa)S_{xyxz}^4 + \upsilon(\lambda,\kappa)S_{zyyy}^4 \\
& + \chi(\lambda,\kappa)S_{yzzz}^4,
\end{aligned}
\tag{5.48}
$$

where all coefficients $\zeta(\lambda,\kappa), \theta(\lambda,\kappa), \ldots, \chi(\lambda,\kappa)$ can be expressed as expansions of the form (5.43) and are real functions of the couplings. Perturbation theory results show that the Hermitian Hamiltonian $h(\lambda,\kappa)$ has the following structure:

$$
\begin{aligned}
h(\lambda,\kappa) = {} & \mu_{xx}^4(\lambda,\kappa)S_{xx}^4 + \nu_{xx}^4(\lambda,\kappa)S_{xux}^4 + \mu_{yy}^4(\lambda,\kappa)S_{yy}^4 + \nu_{yy}^4(\lambda,\kappa)S_{yuy}^4 \\
& + \mu_{zz}^4(\lambda,\kappa)S_{zz}^4 + \nu_{zz}^4(\lambda,\kappa)S_{zuz}^4 + \mu_z^4(\lambda,\kappa)S_z^4 + \mu_{xxz}^4(\lambda,\kappa)\left(S_{xxz}^4 + S_{zxx}^4\right) \\
& + \mu_{xzx}^4(\lambda,\kappa)S_{xzx}^4 + \mu_{yyz}^4(\lambda,\kappa)\left(S_{yyz}^4 + S_{zyy}^4\right) + \mu_{yzy}^4(\lambda,\kappa)S_{yzy}^4 + \mu_{zzz}^4(\lambda,\kappa)S_{zzz}^4 \\
& + \mu_{xxxx}^4(\lambda,\kappa)S_{xxxx}^4 + \mu_{yyyy}^4(\lambda,\kappa)S_{yyyy}^4 + \mu_{zzzz}^4(\lambda,\kappa)S_{zzzz}^4 + \mu_{xxyy}^4(\lambda,\kappa)S_{xxyy}^4 \\
& + \mu_{xyxy}^4(\lambda,\kappa)S_{xyxy}^4 + \mu_{zzyy}^4(\lambda,\kappa)S_{zzyy}^4 + \mu_{zyzy}^4(\lambda,\kappa)S_{zyzy}^4 + \mu_{xxzz}^4(\lambda,\kappa)S_{xxzz}^4 \\
& + \mu_{xzxz}^4(\lambda,\kappa)S_{xzxz}^4.
\end{aligned}
\tag{5.49}
$$

As expected from the expression of q, we find that $h(\lambda,\kappa)$ involves non-local interaction terms proportional to S_{xux}^4, S_{yuy}^4 and S_{zuz}^4. The remaining terms are the natural generalization of the those appearing for the $N = 2, 3$ cases plus additional terms corresponding to interactions that couple all four sites of the chain. Once again, all coefficients $\mu_{xx}^4, \ldots, \mu_{xzxz}^4$ are real functions of the couplings. As for previous cases, it turns out that matrices appearing in the linear combination (5.49) are exactly those that are both invariant under $\mathcal{PT}$-symmetry, according to equation (4.5), and real.

5.5. Some general features from perturbation theory

We would like to end this section by summarizing the main results that we have obtained from our perturbative analysis. Since we have only solved for 2, 3 and 4 sites, our conclusions are based on a case-by-case analysis rather than rigorous proofs. However, we believe that the consistent occurrence of certain features across the various examples that we have studied provides strong support for these conclusions.

Firstly we found that the combination of perturbation theory and the assumption of Hermiticity of the Dyson operator $\eta = e^{q/2}$ fix the metric ρ and therefore the Hermitian Hamiltonian $h(\lambda, \kappa)$ with its corresponding observables *uniquely*. We have established this for $N = 2, 3, 4$ and arbitrary values of both coupling constants as well as for arbitrary N if $\lambda = 0$.

Secondly, concerning the specific algebraic structure of the Hermitian Hamiltonian, we have seen that it becomes more involved for higher values of N. For $N > 2$ it generally includes interaction terms that couple two or more adjacent sites, as well as non-local terms that couple non-adjacent sites. In addition, this structure is entirely dictated by $\mathcal{PT}$ symmetry, which selects out which tensor products of Pauli and identity matrices the Hamiltonian will be a linear combination of. Combining the requirement of $\mathcal{PT}$ symmetry with the requirement of $h(\lambda, \kappa)$ being real completely fixes the general structure of $h(\lambda, \kappa)$, although not the specific dependence on the coupling constants λ and κ, which is fixed by perturbation theory. All examples studied indicate that for a given value of N, all solutions $q_{2k-1}(\lambda)$, with $k \geqslant 0$ at different perturbative orders, share a common structure, namely they are all linear combinations of the same set of matrices, with coefficients that increase in complexity with increasing values of k.

Finally, concerning the numerical accuracy of perturbation theory, we have demonstrated in detail that it converges very quickly for $N = 2$. For $N = 2, 3$ and 4, it becomes very difficult to perform computations up to such high orders of perturbation theory reached for $N = 2$ and the rate of convergence has not been analysed in detail for such cases. An interesting aspect of the model studied here is the dependence of the Hamiltonian on two coupling constants. For $N = 2$, we have carried out perturbation theory in both such couplings and found quick convergence in both cases. All our perturbation theory results suggest that the entries of the Hermitian Hamiltonian $h(\lambda, \kappa)$ can generally be expressed as a double Taylor series in λ and κ.

6. Expectation values of local operators

In this section we want to employ our general formulae in order to compute the expectation values of certain local operators of the chain. In particular, we will be looking at the expectation values of the total spin in the x and z directions in the ground state of the chain. These expectation values are commonly known as the magnetization in the x and z directions. Recalling the results from section 3.2, we define

$$M_z(\lambda, \kappa) = \tfrac{1}{2}\langle \Psi_g | \eta S_z^N \eta | \Psi_g \rangle = \tfrac{1}{2}\langle \psi_g | S_z^N | \psi_g \rangle, \tag{6.1}$$

$$M_x(\lambda, \kappa) = \tfrac{1}{2}\langle \Psi_g | \eta S_x^N \eta | \Psi_g \rangle = \tfrac{1}{2}\langle \psi_g | S_x^N | \psi_g \rangle, \tag{6.2}$$

where $|\psi_g\rangle$ is the ground state of the Hermitian Hamiltonian and $|\Psi_g\rangle$ is the ground state of the non-Hermitian one. We assume that the states are normalized to $\langle \psi_g | \psi_g \rangle = \langle \Psi_g | \Psi_g \rangle = 1$. In the following sections, we will carry out this computation for $\lambda = 0$ with generic N and for $\lambda \neq 0$ for small values of N.
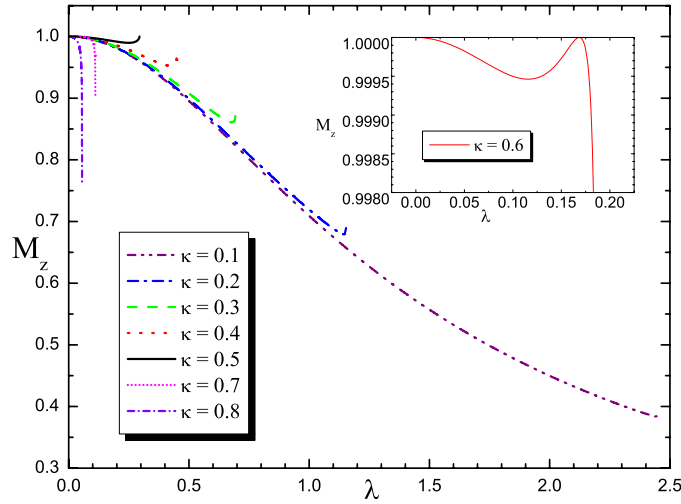
Figure 3. The magnetization in the z-direction for $N = 2$ as a function of λ and κ.

6.1. General solutions for $\lambda = 0$

In section 4.1, we described in detail how for $\lambda = 0$ the original Hamiltonian and its Hermitian counterpart simplify greatly. Indeed, the latter can be found in all generality, for any number of sites, resulting in the expression (4.9). Taking (4.10) and (4.12) into account, it is very easy to show that

$$M_z(0, \kappa) = \frac{N}{2}, \tag{6.3}$$

which is nothing but the total spin of the chain and does not depend on the particular value of the coupling κ. This result is to be expected for a Hamiltonian like (4.9). Naturally, the spins of the chain tend to align in the direction of the field, and will all be up so that the magnetization is just the total spin of the chain and maximal. A similar computation can be performed for $M_x(0, \kappa)$ for each particular value of N. In all cases one finds

$$M_x(0, \kappa) = 0, \tag{6.4}$$

which is also what one would expect for this model, as the Hamiltonian (4.9) does not favour any particular direction of the spin σ_x.

For $\kappa = 0$, the Hamiltonian (1.1) is Hermitian and therefore computations of the magnetization simplify, as $\eta = \mathbb{I}$. The resulting model is well known in the context of integrable models and can be exactly solved as shown for example in [41]. In particular, the magnetization can be obtained exactly for any values of N by using such techniques.

6.2. The $N = 2$ case for $\kappa, \lambda \neq 0$

Let us now compute $M_z(\lambda, \kappa)$ and $M_x(\lambda, \kappa)$ in the more generic situation when both coupling λ and κ are non-vanishing. We will start by analysing the magnetization in the z-direction. In this case ($\lambda \neq 0$), the form of the ground state of the Hermitian chain is not particularly simple and therefore we will work with the first equality in (6.2) and employ the properly normalized ground state of the non-Hermitian Hamiltonian. As figure 3 shows, the magnetization is

maximal at $\lambda = 0$ with value 1, and exhibits different kinds of behaviour as λ increases, depending of the value of κ under consideration.

For every fixed value of κ, the corresponding graph in figure 3 generally only covers a small region of values of λ. These are precisely the values that lie in the region $U_{\mathcal{PT}}$ of figure 1, namely those values for which all eigenvalues of $H(\lambda, \kappa)$ are real. As shown in figure 3, the smaller the value of κ the larger this region becomes in λ. Depending on the value of κ, the magnetization exhibits a rich structure: for $\kappa \geqslant 0.7$ it is a strictly decreasing function, whereas for $\kappa \leqslant 0.6$ it has a minimum. This minimum is located near the critical value of λ above which some eigenvalues of the Hamiltonian become complex, except for $\kappa = 0.6$, where the minimum of the magnetization shifts to a smaller value of λ.

With regard to the magnetization in the x-direction we find that it vanishes for all values of λ and κ. This is so because the Hermitian counter-part of $H(\lambda, \kappa)$ with $N = 2$ has the form (4.29) and therefore the Hamiltonian $h(\lambda, \kappa)$ is invariant under the symmetry $\sigma_i^x \to -\sigma_i^x$ for all i.

We also observe that the magnetization is strictly smaller than 1, as it should be. Computing the expressions (6.1) and (6.2) in the standard metric $\rho = \mathbb{I}$, i.e. disregarding the fact that the Hamiltonian is non-Hermitian, leads to non-physical values larger than 1.

7. Conclusions

We have demonstrated that there are various possibilities to implement $\mathcal{PT}$-symmetry for quantum spin chains, either as a 'macro-reflection' by reflection across the entire chain or as 'micro-reflection' by reflecting at individual sites. These new possibilities constitute symmetries for the model $H(\lambda, \kappa)$ in (1.1) we focussed on, i.e. Ising quantum spin chain in the presence of a magnetic field in the z-direction as well as a longitudinal imaginary field in the x-direction. However, there are also implications for other Hamiltonians such as H_{XXZ} in (2.10) and H_{DG} in (2.12). Due to the various possibilities to implement parity the corresponding metric and therefore the underlying physical model is more ambiguous and it requires further clarification as to which physical system it describes. Remarkably the non-Hermitian Hamiltonian $H(\lambda, \kappa)$ fixes the underlying physics uniquely under the sole assumption that the Dyson map η is Hermitian. As pointed out above, this uniqueness is not obtained in general. One might conjecture that this is due to the finite dimensionality of the Hilbert space, as opposed to continuous models studied for instance in [16, 29], but our comments on H_{XXZ} and H_{DG} suggest this is not the case. The explanation lies surely in the different types of symmetries a Hamiltonian might possess, which is supported by the fact that two different types of metric operators, say ρ and $\hat{\rho}$, can always be used to define a new non-unitary symmetry operator $S = \hat{\rho}\rho^{-1}$ [34, 35].

We have shown that all these possibilities serve to define anti-linear operators, which can not only be used to explain the reality of the spectra and identify the corresponding domains in the coupling constants but can also be employed to define a consistent quantum mechanical framework. Regarding the technical feasibility of this programme, we have demonstrated for two sites that the perturbation theory, in κ as well as in λ, converges very fast by comparing it with the exact result. We took this as encouragement to tackle also three and four sites, albeit up to not as high orders of perturbation theory. Our perturbative analysis has allowed us to demonstrate for specific examples that the combination of perturbation theory and Hermiticity of the Dyson operator are sufficient to uniquely fix η, ρ and $h(\lambda, \kappa)$. In fact, for the model at hand, the constraint of Hermiticity of η appears to be sufficient to entirely fix the algebraic structure of these quantities, even before any perturbative analysis is carried out.

Clearly, there are various open issues and follow-up problems associated with our investigations. Firstly, one may try to complete the analysis for the Hamiltonian $H(\lambda, \kappa)$ by carrying out further numerical studies, perturbative computations for more sites and ultimately obtain a complete analytic understanding for instance by means of the Bethe ansatz. Special attention should be given to the values of κ and λ corresponding to the exceptional points, when the usual analysis is expected to break down. Secondly, one may consider the model for higher spin values as for instance studied in [7]. Finally, it would be also very interesting to investigate some other members of the class belonging to the perturbed $\mathcal{M}_{p,q}$-series of minimal conformal field theories.

Acknowledgments

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