Exact two particle spectrum of the Heisenberg-Peierls chain

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The exact solution for the two particle spectrum of the Heisenberg-Peierls one dimensional spin chain is given by working in the fermionic representation. The resulting equations for the eigenvalues are, in some sense, similar to those of the Richardson’s solution of the BCS model and must be solved numerically.

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I. INTRODUCTION

Low dimensional spin systems have attracted a great deal of interest over the last years because, both, theoretical and experimental reasons. In fact, from the experimental point of view, there are actually many quasi one dimensional compounds such as the organic series \((BCPTTF)\_2X\) with \((X = AsF_6, PF_6)\), the cuprate \(CuGeO_3\) or the \((VO)_2P_2O_7\) compounds, as well as other series as the \(TTFMS_4C_4(CF_3)\_4\) with \(M = Cu, Au, Pt\), or \(Ni\), which can be well described as spin-Peierls chains [1]. Furthermore, we have now the evidence that the two dimensional antiferromagnetism is one of the crucial components of the high temperature superconductivity [2], and we have also Heisenberg spin-ladder compounds which can be viewed as intermediaries between one and two dimensions, and also as between half-integer \((S = 1/2)\) and integer \((S = 0, 1)\) spin chains.

From the theoretical side, these systems are interesting since their low dimensionality makes that their properties are strongly affected by quantum fluctuations and also because of its apparent simplicity. For example, low dimensional electronic materials are known to be very sensitive to structural distortions driven by the electron-phonon interactions which breaks the symmetry of the original (i.e. without electron-phonon interaction) ground state, resulting in a less symmetric but lower energy state, in which the electrons and ions are shifted, from their symmetric positions, in a regular manner that creates a periodic variation of the charge density called charge density wave. This is the famous Peierls instability which
opens a gap at the Fermi surface of the one-dimensional electronic chain, transforming what
would be a metal (in absence of electron-phonon interactions) in a semiconductor. A similar
effect is expected for one dimensional spin chains which are unstable against a dimerized
spin-singlet ground state.

One of the most widely used model for spin interactions is the generalized one dimensional
Heisenberg Hamiltonian which can be written, in terms of the quantum spin operators
\( S_i = (1/2) \sigma_i \) (where \( \sigma_i \) are the Pauli matrices at the site \( i \)), as
\[
H = 4 \sum_{i=1}^{M} J_{i,i+1} S_i S_{i+1},
\]
and that, after some transformations, can be seen also as a one dimensional Hubbard model
for electronic interactions. The case when the coupling \( J_{i,i+1} \) between nearest spins is taken
as a constant is exactly soluble after Bethe and his celebrated Bethe ansatz [3]. Later it was
solved again by applying the Quantum Inverse Scattering methods, with which this model
results inside of a family of solvable models [4]. However the Heisenberg model must be seen
only as a first approximation to the real interactions, as long as a constant coupling between
nearest-neighbors implies that the atoms are taken at fixed positions. If we account for the
vibrations of the atoms, then the coupling between two nearest spins is proportional to the
exchange integral and then it can be written, up to first order, as \( J_{n,n+1} = u - J_1 (v_n - v_{n+1}) \)
where \( u \) and \( J_1 \) are constants and \( v_n \) is the displacement of the \( n \)th atom from its equilibrium
position. In the Born-Oppenheimer approximation, \( v_n = (-1)^n v_0 \) (adiabatic limit) the
Hamiltonian can be written as
\[
H = \sum_{n=1}^{M} (u + (-1)^n v) \sigma_n \sigma_{n+1},
\]
with \( v = 2J_1 v_0 \). The Pauli matrices \( \sigma_n \) act on the two-dimensional space \( \eta_n = C^2 \) whereas
\( H \) acts on the \( 2^M \)-dimensional Hilbert space,
\[
\mathcal{H} = \bigotimes_{n=1}^{M} \eta_n,
\]
which is the tensor product of \( M \) two-dimensional \( C^2 \) spaces. We use periodic boundary
conditions on the lattice with \( M = \) even playing the role of the length of the chain. The
total third component of the spin,
\[
S_3 = \sum_{n=1}^{M} \sigma_n^3
\]
is a conserved magnitude that we shall use to describe the states of the system. In general, to find the exact spectrum of the Hamiltonian (2) is a difficult task and several methods like bosonization [5] and variational [6] have been applied and actually for $v \ll |u|$, case of weak dimerization, the low energy region is believed to be equivalent to that of the Gaussian model [7]. In this paper we want to find the low spin excitations over the state where all $M$ spins are aligned and pointing in the $-Z$ direction (note that the particular direction in which the spins are aligned is not relevant due to the rotational invariance of the Hamiltonian). To do this we shall fermionize the problem with the Jordan-Wigner transformation and use a method analogous to that of the Richardson’s solution [8] of the BCS model of superconductivity.

II. ONE PARTICLE STATES

As said above, our starting point will be an eigenstate of $H$ with all spins aligned in the $-Z$ direction so that it is also an eigenstate of $S_3$ with eigenvalue $-M$; starting from it, we want to find the eigenstates of the Hamiltonian that have one spin flipped in the $+Z$ direction and we call them the one-particle states. The first task is to transform the Hamiltonian (2) in a fermionic Hamiltonian by means of the Jordan-Wigner transformation since, although this is not strictly necessary for these one-particle states, it will be need for the two-particle states, so we start by defining the fermionic operators:

$$a_l = K(l)\sigma_l^-, \quad (5)$$
$$a_l^\dagger = K(l)\sigma_l^+, \quad (6)$$

being $\sigma_l^\pm = (1/2)(\sigma_l^x \pm i\sigma_l^y)$ and

$$K(l) = e^{i\pi \sum_{j=1}^{l-1} \sigma_j^+ \sigma_j^-} = \prod_{j=1}^{l-1}(-\sigma_j^z). \quad (7)$$

These operators are true fermionic operators in the sense that $\{a_l^\dagger, a_m\} = \delta_{l,m}$ and $\{a_l^\dagger, a_m^\dagger\} = 0 = \{a_l, a_m\}$. Furthermore, since

$$\sigma_l^z = 2a_l^\dagger a_l - 1, \quad (8)$$

the total third component of the states is, up to a constant factor, the number operator $N = \sum_{i=1}^{M} a_i^\dagger a_i$, and we can identify the states with $K$ spins flipped with those states that
have $K$ particles of type $a$; furthermore, the total number of fermions is also a conserved quantity. Transforming from the $\sigma$ to the $a$ operators, the Hamiltonian can be written as

$$H = 4 \sum_{l=1}^{M} c_l(u, v) \left( N_l - \frac{1}{2} \right) \left( N_{l+1} - \frac{1}{2} \right)$$

$$+ 2 \sum_{l=1}^{M-1} c_l(u, v) \left( a^\dagger_l a_{l+1} + a^\dagger_{l+1} a_l \right) - 2e^{i\pi N} c_M(u, v) \left( a^\dagger_M a_1 + a^\dagger_1 a_M \right), \quad (9)$$

being $N_l = a^\dagger_l a_l$ and $c_l(u, v) = (u + (-1)^l v)$. Due to the last term, the Hamiltonian reads different depending on the number of particles that has the state on which $H$ acts. However, considering separately the subspaces of even and odd total number of fermions, we may write $H$ in a simple universal way, that is

$$H = uM + 4 \sum_{l=1}^{M} c_l(u, v) \left( N_l N_{l+1} - N_l \right) + 2 \sum_{l=1}^{M} c_l(u, v) \left( a^\dagger_l a_{l+1} + a^\dagger_{l+1} a_l \right) \quad (10)$$

where

$$a_{M+1} = -a_1, \quad a^\dagger_{M+1} = -a^\dagger_1 \quad \text{for states on which $N$ is even}$$

$$a_{M+1} = a_1, \quad a^\dagger_{M+1} = a^\dagger_1 \quad \text{for states on which $N$ is odd}, \quad (11)$$

then, acting on states that have an even number of fermions the Hamiltonian (10) has antiperiodic boundary conditions, whereas the boundary conditions are periodic when $H$ acts on states with an odd number of fermions. Transfomring to momentum space with the Fourier transformation given by

$$b_j = \frac{1}{\sqrt{M}} \sum_{l=1}^{M} e^{ik(j)l} a_l, \quad (12)$$

$$a_l = \frac{1}{\sqrt{M}} \sum_{j=1}^{M} e^{-ik(j)l} b_j, \quad (13)$$

where

$$k(j) = \begin{cases} \frac{2\pi}{M} j & \text{if } m \text{ is odd}, \\ \frac{\pi}{M} (2j - 1) & \text{if } m \text{ is even}, \end{cases} \quad j = 1, \cdots, M$$

and $m$ means the number of fermions of the subspace on which $H$ acts; then the operators $b^\dagger_n$ and $b_n$ create or destroy, respectively, a fermion of momentum $k(n)$ . With these transformations, the Hamiltonian (10) in the momentum space is composed of four pieces, plus the identity times $uM$,

$$H = H_1 + H_2 + H_3 + H_4 + uM \quad (14)$$
where

\begin{align}
H_1 &= -4u \sum_{n=1}^{M} \varepsilon(n) b_n^\dagger b_n, \\
H_2 &= -4iv \sum_{n=1}^{M} \sin(k(n)) b_{n+M/2}^\dagger b_n, \\
H_3 &= -4uM \sum_{n_1,n_2,n_3=1}^{M} e^{i(k(n_3)-k(n_1))} b_{n_1+n_2-n_3}^\dagger b_{n_3} b_{n_2} b_{n_1}, \\
H_4 &= -4vM \sum_{n_1,n_2,n_3=1}^{M} e^{i(k(n_3)-k(n_1))} b_{n_1+n_2-n_3+M/2}^\dagger b_{n_3} b_{n_2} b_{n_1},
\end{align}

and

\begin{equation}
\epsilon(n) = 1 - \cos(k(n)).
\end{equation}

The space of states will be generated now by a vacuum \( |0 \rangle \) with zero excitations, over which act the operators \( b_l^\dagger \) and \( b_l \) that create and destroy excitations that we call particles with momentum \( k(l) \); those states are described by kets of the form \( |l_1, l_2, \ldots, l_m \rangle \) that represents a state of \( m \) particles with momentums \( k(l_1), k(l_2), \ldots, k(l_m) \). Obviously, the total number of particles is conserved by every piece of the Hamiltonian and then we can calculated the energy of the eigenstates with a given number of particles.

The spectrum of energies in the one particle subspace can be obtained easily due to the fact that \( H_1 \) and \( H_2 \) are the only pieces that gives a non null contribution. Acting with \( H \) on the states \( |l \rangle \) and \( |l + M/2 \rangle \), we have

\begin{align}
H_1 |l \rangle &= -4u \epsilon(l) |l \rangle, \\
H_2 |l \rangle &= -4iv \sin(k(l)) |l + M/2 \rangle, \\
H_1 |l + M/2 \rangle &= -4u \epsilon(l + M/2) |l + M/2 \rangle, \\
H_2 |l + M/2 \rangle &= -4iv \sin(k(l + M/2)) |l + M/2 \rangle,
\end{align}

and \( H_3 |l \rangle = H_4 |l \rangle = H_3 |l + M/2 \rangle = H_4 |l + M/2 \rangle = 0 \).

Then we see that the two dimensional subspace generated by the states \( |l \rangle \) and \( |l + M/2 \rangle \) is invariant under the action of \( H \) and consequently the eigenvalues of \( H_1 + H_2 \) are those of the matrix,

\begin{equation}
\begin{pmatrix}
-4ue(l) & 4iv \sin(k(l)) \\
-4iv \sin(k(l)) & -4ue(l + M/2)
\end{pmatrix}.
\end{equation}
and the total energies will be these eigenvalues plus $u M$, i.e.,

$$ E_l^\pm = uM - 4(u \pm \sqrt{(u \cos(k(l))^2 + (v \sin(k(l))^2)}), \quad l = 1, \ldots, \frac{M}{2}, \quad (25) $$

where now $k(l) = (2l\pi/M)$ as corresponds to the subspace with one particle. The corresponding eigenvectors are those of the matrix (24)

$$ v_l^\pm = \frac{1}{n_f^\pm} \begin{pmatrix} i(s_l \pm u \cos(k(l)) \pm v \sin(k(l)) \end{pmatrix}, \quad (26) $$

where $s_l = [u^2 \cos^2(k(l)) + v^2 \sin^2(k(l))]^{1/2}$ and $n_l^\pm = [2s_l^2 \pm 2s_l u \cos(k(l))]^{1/2}$.

### III. TWO PARTICLES STATE CASE

In this case, the pieces of the Hamiltonian $H_3$ and $H_4$ acting on the states are not zero and it does more difficult to find the solution. The states are described by the kets of the form $|l_1, l_2 \rangle$ with, $0 < l_1 < l_2 \leq M$. We can observe that they are eigenstates of $H_1$ and that the action of $H_3$ on them gives new states $|l_1', l_2' \rangle$, in both cases they fulfill the condition $\text{mod}(l_1 + l_2, M) = \text{mod}(l_1' + l_2', M)$. In the same form, the parts $H_2$ and $H_4$ mix the states $|l_1, l_2 \rangle$ with states $|l_1', l_2' \rangle$ being $\text{mod}(l_1 + l_2, M) = \text{mod}(l_1' + l_2' + M/2, M)$. In other words, $H_1$ and $H_3$ conserve the total momentum whereas $H_2$ and $H_4$ change the total momentum by an amount of $\pi$. Then, the subspace generated by states of the form

$$ |\Psi(m) \rangle = \sum_{l=\text{Allpossibles}} g(l, m - l)|l, m - l \rangle, \quad (27) $$

$$ |\Psi(m + M/2) \rangle = \sum_{l=\text{Allpossibles}} h(l, m - l + M/2)|l, m - l + M/2 \rangle, \quad (28) $$

is invariant by the Hamiltonian, and we can reduce to this subspace the problem of finding the eigenvalues and eigenvectors of $H$. Note that in equations (27),(28) the functions $g(l_1, l_2)$ and $h(l_1, l_2)$ are antisymmetric in their arguments, that is $g(l_1, l_2) = -g(l_2, l_1)$ and $h(l_1, l_2) = -h(l_2, l_1)$, in the same way as they are the fermionic states $|l_1, l_2 \rangle = -|l_2, l_1 \rangle$.

#### A. Case $u = 0$

Let us begin with the case $u = 0$. Then the total Hamiltonian has only the alternating term so the equations are simpler and we can see better the method. Working in units of $v$
(or \( v = 1 \)) and taking

\[
\Xi(m) = i\psi(m) + \psi(m + M/2),
\]

(29)

and demanding that \((H_2 + H_4) \Xi(m) = E \Xi(m)\) we obtain that

\[
E [g(l, m - l) - g(m - l, l)] =
\]

\[
8 \left\{ 2B(m) \sin [k(l - m/2)] + \frac{1}{2} \sin [k(l)] (h(l - M/2, m - l) - h(m - l, l + M/2)) + \sin [k(m - l)] (h(l, m - l + M/2) - h(m - l - M/2, l)) \right\}, \quad (30)
\]

and

\[
E [h(l, m - l + M/2) - h(m - l + M/2, l)] = 8 \left\{ 2A(m) \cos [k(l - m/2)] + \frac{1}{2} \sin [k(l)] (g(m - l + M/2, l - M/2) - g(l - M/2, m - l + M/2)) + \sin [k(m - l)] (g(l, m - l) - h(m, l)) \right\}, \quad (31)
\]

where \( A(m) \) and \( B(m) \) are defined as

\[
A(m) = \frac{1}{M} \sum_l \sin [k(l - m/2)] g(l, m - l), \quad (32)
\]

\[
B(m) = \frac{1}{M} \sum_l \cos [k(l - m/2)] h(l, m - l + M/2). \quad (33)
\]

These equations (30) and (31) can be solved for \( g \) and \( h \). After a rather tedious calculus we have obtained the solutions for \( g(l_1, l_2), h(l_1, l_2) \) and the eigenvalues \( E \) in the form

\[
h(l_1, l_2) = \frac{8EA(l_1 - l_2) \cos [k((l_1 - l_2 + M)/2)]}{D_1(E, l_1, l_2)} + \frac{64B(l_1 - l_2) \sin [k((l_1 + l_2 + M)/2)] \sin [k((l_1 - l_2 + M)/2)] \cos [k((l_1 - l_2 + M)/2)]}{D_2(E, l_1, l_2)},
\]

\[
g(l_1, l_2) = \frac{8EB(l_1 - l_2) \sin [k((l_1 - l_2)/2)]}{D_1(E, l_1, l_2)} - \frac{64A(l_1 - l_2) \cos [k((l_1 + l_2)/2)] \sin [k((l_1 - l_2)/2)] \cos [k((l_1 - l_2)/2)]}{D_2(E, l_1, l_2)}, \quad (34)
\]

where the functions \( D_i(E, l_1, l_2) \) are defined as

\[
D_i(E, l_1, l_2) = E^2 - 16 \left[ \sin(k(l_1)) - (-1)^i \sin(k(l_2)) \right]^2, \quad (i=1,2), \quad (35)
\]

and the eigenvalues \( E \) depend only on the total momentum of the state \( m = l_1 + l_2 \), and for each value of \( m \) satisfy the consistency equation

\[
\left( \frac{8E}{M} \right)^2 \left( \sum_l \frac{\cos^2 [k(l - m/2)]}{D_1(E, l, m - l)} \right) \left( \sum_l \frac{\sin^2 [k(l - m/2)]}{D_2(E, l, m - l)} \right) = 1. \quad (36)
\]
Notice that (36) is quadratic in the energy $E$ and hence it gives symmetric eigenvalues $\pm E$ as corresponds to the charge conjugation symmetry of the Hamiltonian. Note that this consistency equation (36) is of the type of the eigenvalue equation for the Richardson’s solution for the BCS model [8], so the study of the completeness of the solution is analogous to that of this model.

![Graphical solution of the equation (36) for $m = 3$ and $M = 12$. Dashed line corresponds to the $G(E) = (8E/M)^{-2}$ term and the continuous line is $F(E)$.](image)

Figure 1: Graphical solution of the equation (36) for $m = 3$ and $M = 12$. Dashed line corresponds to the $G(E) = (8E/M)^{-2}$ term and the continuous line is $F(E)$.

As an example, in Fig. (1) we plot the graphical solution of Eq. (36) for the case $M = 12$ and $m = 3$; there we plot the curves $G(E) = (8E/M)^{-2}$ and $F(E) = \left(\sum_l \frac{\cos^2[k(l-m/2)]}{D_1(E,l,m-l)}\right) \left(\sum_l \frac{\sin^2[k(l-m/2)]}{D_2(E,l,m-l)}\right)$. Here it is evident that the number of solutions is determined by the discontinuities of the function $F(E)$ along the positive axis.

**B. General case**

Now we return to the general case when $u$ and $v$ are $\neq 0$. The action of the different parts of the Hamiltonian on the states (27 - 28) is given by,

$$H_1|\psi(m \ )> = -4u \sum_l (\varepsilon(l) + \varepsilon(m-l)) g(l, m-l) |l, m-l >,$$

$$H_1|\psi(m + M/2) > = -4u \sum_l (\varepsilon(l) + \varepsilon(m-l + M/2))$$

(37)
\[ h(l, m - l + M/2) |l, m - l + M/2 >, \] (38)

\[ H_2 |\psi(\ ) > = -4iv \sum_l (\sin(k(l)) g(l - M/2, m - l + M/2) \]
\[ + \sin(k(m - l)) g(l, m - l)) |l, m - l + M/2 >, \] (39)

\[ H_2 |\psi(m + M/2) > = 4iv \sum_l (\sin(k(l)) h(l - M/2, m - l) \]
\[ + \sin(k(m - l)) h(l, m - l + M/2)) |l, m - l >, \] (40)

\[ H_3 |\psi(\ ) > = 16uA(m) \sum_l \sin(k(l) - s(m)/2) |l, m - l >, \] (41)

\[ H_3 |\psi(m + M/2) > = 16uB(m) \sum_l \cos(k(l) - s(m)/2) |l, m - l + M/2 >, \] (42)

\[ H_4 |\psi(\ ) > = 16ivA(m) \sum_l \cos(k(l) - s(m)/2) |l, m - l + M/2 >, \] (43)

\[ H_4 |\psi(m + M/2) > = 16ivB(m) \sum_l \sin(k(l) - s(m)/2) |l, m - l >, \] (44)

being now

\[ A(m) = \frac{1}{M} \sum_l \sin(k(l) - s(m)/2)g(l, m - l), \] (45)

\[ B(m) = \frac{1}{M} \sum_l \cos(k(l) - s(m)/2)h(l, m - l + M/2), \] (46)

and

\[ s(m) = \frac{2\pi}{M}(m - 1). \] (47)

The sums are understood to all different values of the index and the integer labels of the states are module M.

The energies will be obtained from the compatibility of the eigenvalue equation

\[ (H_1 + H_2 + H_3 + H_4)(\Psi(m) + \Psi(m + M/2)) = E (\Psi(m) + \Psi(m + M/2)). \] (48)

Equating the coefficients of every state in the first member and in the second member, we can observe that the relations between them mix only the \(g(l, m - l), g(l - M/2, m - l + M/2), h(l - M/2)\) and \(h(l - M/2, m - l)\) terms, besides of the functions \(A(m)\) and \(B(m)\) that depends of all coefficients. This relations are expressed as the system of linear equations,

\[
(EI - M) \begin{pmatrix}
g(l, m - l) \\
g(l - M/2, m + M/2 - l) \\
h(l, m + M/2 - l) \\
h(l + M/2, m - l)
\end{pmatrix} = 16 \begin{pmatrix}
\sin(k(l) - s(m)/2)(uA(m) + ivB(m)) \\
- \sin(k(l) - s(m)/2)(uA(m) + ivB(m)) \\
\cos(k(l) - s(m)/2)(-ivA(m) + uB(m)) \\
- \cos(k(l) - s(m)/2)(-ivA(m) + uB(m))
\end{pmatrix}
\] (49)
where \( \mathbf{M} \) is the matrix

\[
\mathbf{M} = \begin{pmatrix}
d_1(l, m) & 0 & c_1(l, m) & c_2(l, m) \\
0 & d_1(l - \frac{M}{2}, m) & -c_2(l, m) & -c_1(l, m) \\
-c_1(l, m) & c_2(l, m) & d_2(l, m) & 0 \\
-c_2(l, m) & c_1(l, m) & 0 & d_2(l - \frac{M}{2}, m)
\end{pmatrix}
\]

with

\[
c_1(l, m) = 4iv \sin(k(m - l)) ,
\]
\[
c_2(l, m) = 4iv \sin(k(l)) ,
\]
\[
d_1(l, m) = -4u(\varepsilon(l) + \varepsilon(m - l)) ,
\]
\[
d_2(l, m) = -4u(\varepsilon(l) + \varepsilon(m - l + \frac{M}{2})) .
\]

From the equations (51), we can get the solutions of \( g(l, m - l) \) and \( h(l, m - l + \frac{M}{2}) \) by making use of the inverse matrix of \( (E \mathbf{I} - \mathbf{M}) \). The matrix elements of that matrix are function of the \( l, m \), and the eigenvalues \( E \) of the Hamiltonian \( H = H_1 + H_2 + H_3 + H_4 \). If we call \( s_{i,j} \) to the matrix elements of \( (E \mathbf{I} - \mathbf{M})^{-1} \) we obtain,

\[
g(l, m - l) = 16(\cos(k(l) - \frac{s(m)}{2})(s_{1,3} - s_{1,4})(-ivA(m) + uB(m)) + \sin(k(l) - \frac{s(m)}{2})(s_{1,1} - s_{1,2}))(uA(m) + ivB(m)) ,
\]
\[
h(l, m - l + \frac{M}{2}) = 16(\cos(k(l) - \frac{s(m)}{2})(s_{3,3} - s_{3,4})(-ivA(m) + uB(m) + \sin(k(l) - \frac{s(m)}{2})(s_{3,1} - s_{3,2}))(uA(m) + ivB(m)) ,
\]

where the \( s \) functions are

\[
s_{11} = \frac{1}{D} c_1(l, m)^2 (E - d_2(l, m)) + \\
\frac{1}{D} \left( c_2(l, m)^2 + \left( E - d_1(l - \frac{M}{2}, m) \right) (E - d_2(l, m)) \right) \left( E - d_2(l - \frac{M}{2}, m) \right)
\]
\[
s_{12} = \frac{1}{D} c_1(l, m) c_2(l, m) \left( 2E - d_2(l, m) - d_2(l - \frac{M}{2}, m) \right)
\]
\[
s_{13} = \frac{1}{D} c_1(l, m) \left( c_1(l, m)^2 - c_2(l, m)^2 + \left( E - d_1(l - \frac{M}{2}, m) \right) (E - d_2(l - \frac{M}{2}, m)) \right)
\]
\[
s_{14} = \frac{1}{D} c_2(l, m) \left( -c_1(l, m)^2 + c_2(l, m)^2 + \left( E - d_1(l - \frac{M}{2}, m) \right) (E - d_2(l, m)) \right)
\]
\[
s_{22} = \frac{1}{D} (E - d_2(l, m)) \left( c_2(l, m)^2 + (E - d_1(l, m)) \left( E - d_2(l - \frac{M}{2}, m) \right) \right) + 
\]
\[
\frac{1}{D} c_1(l, m)^2 \left( E - d_2 \left( l - \frac{M}{2}, m \right) \right)
\]

\[
s_{23} = \frac{1}{D} c_2(l, m) \left( c_1(l, m)^2 - c_2(l, m)^2 - (E - d_1(l, m)) \left( E - d_2(l - \frac{M}{2}, m) \right) \right)
\]

\[
s_{24} = \frac{1}{D} c_1(l, m) \left( -c_1(l, m)^2 + c_2(l, m)^2 - (E - d_1(l, m)) \left( E - d_2(l, m) \right) \right)
\]

\[
s_{33} = \frac{1}{D} c_1(l, m)^2 \left( E - d_1(l, m) \right) + \frac{1}{D} \left( E - d_1(l - \frac{M}{2}, m) \right) \left( c_2(l, m)^2 + (E - d_1(l, m)) \left( E - d_2(l - \frac{M}{2}, m) \right) \right)
\]

\[
s_{34} = \frac{1}{D} c_1(l, m) c_2(l, m) \left( -2 E + d_1(l, m) + d_1(l - \frac{M}{2}, m) \right)
\]

\[
s_{44} = \frac{1}{D} c_1(l, m)^2 \left( E - d_1(l - \frac{M}{2}, m) \right) + \frac{1}{D} \left( E - d_1(l, m) \right) \left( c_2(l, m)^2 + \left( E - d_1(l - \frac{M}{2}, m) \right) \left( E - d_2(l, m) \right) \right)
\]

(57)

being \( D \) the determinant of \( E \mathbf{1} - \mathbf{M} \), i.e., the characteristic polynomial of \( \mathbf{M} \)

\[
D = c_1(l, m)^2 \left( c_1(l, m)^2 - c_2(l, m)^2 + (E - d_1(l, m)) \left( E - d_2(l, m) \right) \right)
\]

\[
+ c_2(l, m)^2 \left( -c_1(l, m)^2 + c_2(l, m)^2 + \left( E - d_1(l - \frac{M}{2}, m) \right) \left( E - d_2(l, m) \right) \right)
\]

\[
+ \left( c_2(l, m)^2 \left( E - d_1(l, m) \right) + \left( E - d_1(l - \frac{M}{2}, m) \right) \left( c_1(l, m)^2 + (E - d_1(l, m)) \left( E - d_2(l, m) \right) \right) \right) \left( E - d_2(l - \frac{M}{2}, m) \right)
\]

(58)

With the last expressions, we can substitute \( g(l, m - l) \) and \( h(l, m - l + M/2) \) given by equations (55)-(56) in the definitions for \( A(m) \) and \( B(m) \) given in the equations (14,16). If we call

\[
c_{1,1}(m, E) = \frac{16}{M} \sum_l \sin(k(l) - \frac{s(m)}{2}) \cos(K(l) - \frac{s(m)}{2})(s_{1,3} - s_{1,4}),
\]

(59)

\[
c_{1,2}(m, E) = \frac{16}{M} \sum_l \sin(k(l) - \frac{s(m)}{2})^2(s_{1,1} - s_{1,2}),
\]

(60)

\[
c_{2,1}(m, E) = \frac{16}{M} \sum_l \cos(k(l) - \frac{s(m)}{2})^2(s_{3,3} - s_{3,4}),
\]

(61)

\[
c_{2,2}(m, E) = \frac{16}{M} \sum_l \sin(k(l) - \frac{s(m)}{2}) \cos(K(l) - \frac{s(m)}{2})(s_{3,1} - s_{3,2}),
\]

(62)

Then we obtain the equations

\[
A(m) = c_{1,1}(m, E)(-\nu A(m) + uB(m)) + c_{1,2}(m, E)(uA(m) + \nu B(m))
\]

(63)

\[
B(m) = c_{2,1}(m, E)(-\nu A(m) + uB(m)) + c_{2,2}(m, E)(uA(m) + \nu B(m)).
\]

(64)
The compatibility of that system impose the condition,
\[
\begin{vmatrix}
-ivc_{1,1}(m, E) + uc_{1,2}(m, E) - 1 & uc_{1,1}(m, E) + ivc_{1,2}(m, E) \\
-ivc_{2,1}(m, E) + uc_{2,2}(m, E) & uc_{2,1}(m, E) + ivc_{2,2}(m, E) - 1
\end{vmatrix} = 0,
\]
(65)
this equation plays the role of the Bethe ansatz equations and it can be solved by algebraic or numerical methods for any \(1 \leq m \leq M\) and an arbitrary number of sites \(M\).

The determinant \(D\) is the four degree characteristic polynomial of the matrix \(M\) that correspond to the Hamiltonian piece \(H_{12} = H_1 + H_2\). It is factorized as the product
\[
D(E) = \prod_{i=1}^{4} (E - E_i)
\]
(66)
where \(E_i\) are the eigenvalues of \(H_{12}\). In some cases it can happen that some of this factors will be common to all numerators of the functions \(g\) and \(h\) involved in the same set of equations (69). Then, the corresponding eigenvalue \(E_i\) of \(H_{12}\) will be also eigenvalue of the total Hamiltonian, i.e., solution of (65). Due to that, we must take care since that eigenvalue will not appear if we do the simplification in the expressions for the \(g\) and \(h\) functions.

For small \(M\) the solutions of the equation (65) can be compared with the solutions obtained after diagonalizing the total Hamiltonian in both, the site space or the momentum space. For example, for \(M = 6\) we have that the dimension of the state space is 15 whereas the invariant subspace generate by the states with \(m\) and \(m + M/2\) has 5 dimensions. The solutions can be obtained by algebraic methods in the two cases. Using the Mathematica application, for \(m = 1\), we obtain in the two cases the solutions
\[
E = 0
\]
(67)
\[
E = -8 u
\]
(68)
\[
E = -8 u + \frac{16}{(12)^{1/3}} \frac{(u^2 + v^2)}{f(u, v)} + 2 \left( \frac{2}{3} \right)^{\frac{4}{3}} f(u, v)
\]
(69)
\[
E = -8 u - \frac{8 \left(1 + i \sqrt{3}\right)}{(12)^{1/3}} \frac{(u^2 + v^2)}{f(u, v)} - \left( \frac{2}{3} \right)^{\frac{4}{3}} \left(1 - i \sqrt{3}\right) f(u, v)
\]
(70)
\[
E = -8 u - \frac{8 \left(1 - i \sqrt{3}\right)}{(12)^{1/3}} \frac{(u^2 + v^2)}{f(u, v)} - \left( \frac{2}{3} \right)^{\frac{4}{3}} \left(1 + i \sqrt{3}\right) f(u, v),
\]
(71)
where \(f(u, v)\) is defined as
\[
f(u, v) = \left(-9u(u^2 - v^2) + \sqrt{3} \sqrt{-5 u^6 - 150 u^4 v^2 - 69 u^2 v^4 - 32 v^6}\right)^{\frac{1}{3}}
\]
(72)
The solution $E = -8u$ is also eigenvalue of $H_{12}$. Numerical evaluations show that these solutions are real as correspond to an selfadjoint Hamiltonian.

It is interesting to get the values of the energies for the special cases $v = 0$ and $u = 0$. In the first case, we obtain obviously the spectrum of the $XXX$-Heisenberg model and the equations (19) become very simple since $H_1$ is diagonal and $H_2$ is null. In the second case, $u = 0$, the equations (19) are simplified considerably too, since now the functions $d$ are null. In both cases the solutions are,

\begin{align}
E_{v=0} &= \{0, -8u, -4u, 2(-5 + \sqrt{5})u, -2(5 + \sqrt{5})u\}, \\
E_{u=0} &= \{0, 0, 0, 4\sqrt{2}v, -4\sqrt{2}v\},
\end{align}

that have been obtained from (67 - 71) by making use of the respective substitutions for $u$ and $v$.

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