

# On the completeness of the set of Bethe-Hulthén solutions of the linear Heisenberg system

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**Abstract.** In this work we formulate the standard form of the solutions of the Heisenberg chain with periodic boundary conditions and show that these solutions can be transformed into the well-known Bethe-Hulthén solutions. The standard form is found by solving the secular problem, separated according to the irreducible representations of the translation group. The relevant parameters  $\exp(ik_j)$  of the Bethe-Hulthén solutions are found from a set of linear equations with coefficients derived from the standard solutions. This correspondence between standard and Bethe-Hulthén solutions realizes the completeness of the Bethe-Hulthén method.

## 1. Introduction

In our contribution to SSPCM 2002 [1] we already gave a historic overview of papers related to the epoch-making work of Bethe [2] and Hulthén [3]. In this work we will derive an algebraic method to determine the relevant parameters of the Bethe-Hulthén (B.H.) solutions:

$$k_j \text{ or } x_j = e^{ik_j}. \quad (1)$$

This derivation will start from a solution in the standard form, i.e. a solution found by a straightforward diagonalization of the linear Heisenberg problem. In this way we give a proof of the existence of the B.H. solutions together with a set of algebraic equations for the parameters  $e^{ik_j}$ . The solutions in standard form are given for the linear Heisenberg problem with periodic boundary conditions and an isotropic interaction between nearest neighbour interactions in the chain.

This standard solution is given in terms of an amplitude for all the spin configurations, i.e.: Ising states, for an arbitrary chosen z-axis. Ising states are the eigenstates of the z components of all individual spins. From translational symmetry it follows that all solutions may be chosen to correspond to an irreducible representation of the translation group. All Ising states for one stationary state have the same number of inverted spins with respect to the ferromagnetic state, for which all z-components of the individual spins have the value  $1/2\hbar$ . So we may characterize all these Ising states for a stationary state with  $r$  deviations in a ring of  $N$  spins, by the relative positions of the inversions and the position of one inversion. The corresponding amplitude factorizes in the following way:

$$e^{ik_j} c(d_1, d_2, \dots, (d_r)) \quad (2)$$

in which the  $d_j (j = 1, 2, \dots, r)$  are the distances between the successive deviations at positions  $j_1, j_2, \dots, j_r$  :

$$\begin{aligned} d_1 &= j_2 - j_1, d_2 = j_3 - j_2, \dots, d_r = N + j_1 - j_r, \\ 1 &\leq j_1 < j_2 < j_3 < \dots < j_{r-1} < j_r \leq N. \end{aligned} \quad (3)$$

The special form of the expression for the distance  $d_r$  reflects the periodic boundary conditions. The "wave number"  $k$  characterizes the irreducible representation of the translation group to which the stationary state belongs.

In identifying each stationary state in the standard form with a state in the B.H.-representation the amplitudes  $c(d_1, d_2, \dots, (d_r))$  will be written in terms of the  $x_j$  ( $j = 1, \dots, r$ ) of the corresponding B.H.-state. The question to be solved in this paper is whether or not this is always possible. The identification results in a set of linear equations for the elementary symmetric polynomials of the parameters  $x_j$ , which determine a unique solution for these parameters, apart from an irrelevant permutation.

The following section is devoted to description of the standard solution. Sections 3 and 4 contain an exposé of the Bethe-Hulthén solution for two different cases: First we give in section 3 a description of the normal case, i.e. the case in which there are no bound pairs, whereas in section 4 the solutions contain one bound pair. Solutions with more than one bound pair do not exist. These sections also give a method to determine the B.H.-parameters starting from the standard solution. In the final sections 5 and 6 we give some examples of our method.

## 2. Standard solutions for the Heisenberg chain.

The general form of the stationary states for given number of deviations  $r$  and a given representation of the translation group is given by:

$$\begin{aligned} \Psi_{k,r,n} &= \sum_{j=1}^{N-r+1} \sum_{d_1=1}^{N-j-r+2} \sum_{d_2=1}^{N-j-d_1-r+3} \dots \sum_{d_{r-1}=1}^{N-j-d_1-d_2-\dots-d_{r-2}} e^{ikj} \times \\ &\times c(d_1, d_2, d_3, \dots, d_{r-1}, (N - d_1 - d_2 - d_3 - \dots - d_{r-1})) \times \\ &\times \Phi_{j \ j+d_1 \ j+d_1+d_2 \ \dots \ j+d_1+d_2+\dots+d_{r-1}} \end{aligned} \quad (4)$$

$$\begin{aligned} k &= \frac{2\pi\lambda}{N} \\ \lambda &= -\frac{N}{2}, -\frac{N}{2} + 1, \dots, \frac{N}{2} - 1 \quad (N \text{ even}) \\ \lambda &= -\frac{N-1}{2}, -\frac{N-3}{2}, \dots, \frac{N-1}{2} \quad (N \text{ odd}) \end{aligned} \quad (5)$$

$$\begin{aligned} &\Phi_{j \ j+d_1 \ j+d_1+d_2 \ \dots \ j+d_1+d_2+\dots+d_{r-1}} \\ &= S_j^- S_{j+d_1}^- S_{j+d_1+d_2}^- \dots S_{j+d_1+d_2+\dots+d_{r-1}}^- | + + + \dots + \rangle \end{aligned} \quad (6)$$

in which  $S_l^-$  ( $l = 1, 2, 3, \dots, N$ ) represents the lowering operators:

$$S_l^- = S_{l,x} - iS_{l,y} \quad (l = 1, 2, 3, \dots, N). \quad (7)$$

The index  $n$  is used to distinguish between states corresponding with the same  $k$  and  $r$ .

The ferromagnetic or "pseudo vacuum" state is given by:

$$| + + + \dots + \rangle \quad (8)$$

$$S_{l,z} | +++ \dots + \rangle = \frac{1}{2} | +++ \dots + \rangle \quad (\hbar = 1) \quad (l = 1, 2, 3 \dots N). \quad (9)$$

Periodic boundary conditions result in stationary states corresponding with a given irreducible representation of the translation group:

$$\begin{aligned} & c(d_1, d_2, d_3, \dots, d_{r-1}, (N - d_1 - d_2 - d_3 - \dots - d_{r-1})) \\ = & e^{ikd_1} c(d_2, d_3, \dots, d_{r-1}, N - d_1 - d_2 - d_3 - \dots - d_{r-1}, (d_1)) \end{aligned} \quad (10)$$

$$d_r = N - d_1 - d_2 - d_3 - \dots - d_{r-1}. \quad (11)$$

The Hamiltonian of the Heisenberg chain (cf. W.J. Caspers e.a. Proc. SSPCM 2000 [5]) has the following symmetries: translational invariance, rotational invariance in spin space, time-reversal symmetry. The first symmetry implies that  $k$  is a good quantum number (already used in the representation of the stationary states in (4)). The second and third symmetry imply that we may restrict ourselves to the consideration of the stationary states with:  $r = N/2$  ( $N$  even) or  $r = (N - 1)/2$  ( $N$  odd). Stationary states with different  $r$  may be derived from these by a rotation in spin space or time reversal, or a combination of both operations.

In the following sections we give the transformation of the standard solution into the B.H.-representation, which results in a set of equations for the **symmetrized products** of the parameters  $x_n = e^{ik_n}$  in terms of the amplitudes of the standard solution:

$$c(d_1, d_2, d_3, \dots, d_{r-1}, (N - d_1 - d_2 - d_3 - \dots - d_{r-1})).$$

In section 3 this is done for the case without bound pairs and in section 4 for the case with one bound pair, covering in this way all possibilities.

The set of parameters  $x_n$  (or  $k_n$ ) in the first case equals  $r = [N/2]$ , whereas in the second case the number of  $x_n$  to be determined equals:  $r - 2 = N/2 - 2$  ( $N$  is even), one pair of deviations being bound into a pair on neighbouring positions in the chain, the pair having a resulting wave number  $K_0 = -\pi$ .

### 3. Bethe-Hulthén representation for states without a bound pair

The B.H.-solutions for given  $k$  and  $r$  has the form:

$$\begin{aligned} \Omega_{k,r,m} = & \sum_{1 \leq j_1 < j_2 < j_3 < \dots < j_r \leq N} \sum_P e^{i(\sum_{l=1}^r k_{P(l)} j_l + \frac{1}{2} \sum_{l < p} \phi_{P(l)P(p)})} \times \\ & \times \Phi_{j_1 j_2 j_3 \dots j_r} \end{aligned} \quad (12)$$

with:

$$2 \cot\left(\frac{\phi_{lp}}{2}\right) = \cot\left(\frac{k_l}{2}\right) - \cot\left(\frac{k_p}{2}\right), \phi_{lp} = -\phi_{pl} \quad (13)$$

$$\sum_{l=1}^r k_l = k \quad (14)$$

in which formulas we have replaced the numbering of the deviations in (4) :  $(j, j + d, j + d_1 + d_2, \dots, j + d_1 + d_2 + \dots + d_{r-1})$  by:  $(j_1, j_2, j_3, \dots, j_r)$ . The symbol  $P$  stands for a permutation of the indices:  $1, 2, \dots, r$ . The individual wave numbers of the  $r$  deviations constitute the solution of a set of the B.H.-equations given in ref. 5. The question to be answered is whether or not such a B.H.-solution exists corresponding to a given standard solution. In general there are more solutions of the form (12) for given  $k$  and  $r$ , so we need an additional index  $m$ . The set of wave

numbers does not contain identical  $k_l = k_p$  because the state vector vanishes for this case, with the exception of  $k_l = 0$ , which may occur in arbitrary multiplicity. Apart from this condition there is the restriction that the wave numbers are real or appear in complex conjugated pairs.

Now we may rewrite (12) in the equivalent form:

$$\Omega_{k,r,m} = e^{i\frac{1}{2}\sum_{l<p}\phi_{lp}} \sum_{1\leq j_1<j_2<j_3<\dots<j_r\leq N} \sum_P e^{i(\sum_{l=1}^r k_{P(l)}j_l + \sum_{p<q, P(p)>P(q)}\phi_{P(p)P(q)})} \Phi_{j_1j_2j_3\dots j_r}. \quad (15)$$

The alternative set of parameters:

$$e^{ik_l} = x_l, \quad e^{i\phi_{pq}} = -\frac{2x_p - x_p x_q - 1}{2x_q - x_p x_q - 1} \quad (16)$$

result in the following form of the state vector  $\Theta_{k,r,m}$ , apart from a trivial factor:

$$\Theta_{k,r,m} = \sum_{1\leq j_1<j_2<j_3<\dots<j_r\leq N} \sum_P \prod_{l=1}^r x_{P(l)}^{j_l} \prod_{\substack{p<q \\ P(p)>P(q)}} \left( -\frac{2x_{P(p)} - x_{P(p)}x_{P(q)} - 1}{2x_{P(q)} - x_{P(p)}x_{P(q)} - 1} \right) \times \Phi_{j_1j_2j_3\dots j_r} \quad (17)$$

The relation between the standard form of a solution and its B.H.-representation now follows from (4) and (17):

$$\begin{aligned} & c(d_1, d_2, d_3, \dots, d_{r-1}, (d_r)) \\ &= \sum_P \prod_{l=2}^r x_{P(l)}^{d_1+d_2+\dots+d_{l-1}} \prod_{\substack{p<q \\ P(p)>P(q)}} \left( -\frac{2x_{P(p)} - x_{P(p)}x_{P(q)} - 1}{2x_{P(q)} - x_{P(p)}x_{P(q)} - 1} \right) \\ d_r &= N - d_1 - d_2 - d_3 \dots - d_{r-1}. \end{aligned} \quad (18)$$

The coefficients  $c(d_1, d_2, d_3, \dots, d_{r-1}, (d_r))$  of (15) may be rewritten:

$$c(d_1, d_2, d_3, \dots, d_{r-1}, (d_r)) = \left( \prod_{l<p} \frac{x_l - x_p}{2x_l - x_l x_p - 1} \right) \times B(d_1, d_2, d_3, \dots, d_{r-1}, (d_r)) \quad (19)$$

in which equation  $B(d_1, d_2, d_3, \dots, d_{r-1}, (d_r))$  is a *symmetric polynomial* in terms of  $(x_1, x_2, \dots, x_r)$ , which may be expressed in terms of the elementary symmetric polynomials ESP:

$$\begin{aligned} A_1 &= -\sum_{l=1}^r x_l, \quad A_2 = \sum_{1\leq l<p\leq N} x_l x_p, \quad A_3 = -\sum_{1\leq l<p<q\leq N} x_l x_p x_q, \dots \\ A_r &= (-)^r x_1 x_2 \dots x_r. \end{aligned} \quad (20)$$

The parameters  $x_l$  now obey the equation:

$$x^r + A_1 x^{r-1} + A_2 x^{r-2} + \dots + A_r = 0. \quad (21)$$

The coefficients  $c(d_1, d_2, d_3, \dots, d_{r-1}, (d_r))$  and  $B(d_1, d_2, d_3, \dots, d_{r-1}, (d_r))$  obey identical periodic boundary conditions, which for the last read:

$$B(d_1, d_2, d_3, \dots, d_{r-1}, (d_r)) = e^{ikd_1} B(d_2, d_3, d_4, \dots, d_r, (d_1)). \quad (22)$$

Now it turns out that (18) gives the possibility to formulate linear equations for the ESP in terms of the amplitudes of a given solution in the standard form. It can be seen from the form of this equation that multiplication of the right member by one of the ESP results in linear combination of similar expressions for different sets of distances  $(d'_1, d'_2, d'_3, \dots, d'_{r-1}, (N - d'_1 - d'_2 - d'_3 - \dots - d'_{r-1}))$ . One of these  $r$  distances, however, may turn out to have the value 0. Such a set of distances could not possibly correspond to an amplitude in the standard representation, so it should be eliminated by taking a suitable linear combination of possible products of these right members and ESP. This procedure will be illustrated in section 5, in which some examples will be given.

#### 4. Bethe-Hulthén representation for states with one bound pair

Formally a bound pair may be considered to correspond to a set of wave numbers:

$$k_1 = -\frac{\pi}{2} - i\delta, \quad k_2 = -\frac{\pi}{2} + i\delta \quad (\delta \Rightarrow \infty) \quad (23)$$

which should be combined with a regular set of finite, but generally complex wave numbers:

$$k_3, k_4, \dots, k_r. \quad (24)$$

This set contains only complex conjugated pairs or real  $k_l$ . There does not exist degeneracy in the spectrum of wave numbers, because this will result in a vanishing (non-physical) state vector, with the exception of zero wave numbers.

A complete set of wave numbers for this case is given by:

$$K_0 = -\pi, k_3, k_4, \dots, k_r \quad (25)$$

in which  $K_0$  represents the bound pair.

It can be shown that there are no larger groups of bound deviations and that also the combination of 2 bound pairs is forbidden, because these configurations result in boundary conditions that cannot be fulfilled.

Now we may formulate an equivalent form of (15) for a stationary state with one bound pair, after we have determined the phase shift  $\phi_{0l}$  for the interchange of the bound pair with one of the individual  $k_p$  ( $p = 3, 4, \dots, r$ ). This phase shift follows from (15) for the consecutive interchange of deviations with  $k_1$  and  $k_2$  of the form given in (23) and a third with wave number  $k_p$ , the resulting expression taken in the limit  $\delta \Rightarrow \infty$ :

$$\begin{aligned} e^{i\phi_{0l}} &= \lim_{\delta \Rightarrow \infty} \frac{2e^{i(-\frac{\pi}{2}-i\delta)} - e^{i(-\frac{\pi}{2}-i\delta)}e^{ik_l} - 1}{2e^{ik_l} - e^{i(-\frac{\pi}{2}-i\delta)}e^{ik_l} - 1} \frac{2e^{i(-\frac{\pi}{2}+i\delta)} - e^{i(-\frac{\pi}{2}+i\delta)}e^{ik_l} - 1}{2e^{ik_l} - e^{i(-\frac{\pi}{2}+i\delta)}e^{ik_l} - 1} \\ &= \frac{2 - e^{ik_l}}{-e^{ik_l}} \frac{-1}{2e^{ik_l} - 1} = \frac{2 - x_l}{x_l(2x_l - 1)} \quad (l = 3, 4, \dots, r). \end{aligned} \quad (26)$$

Using the value of the phase shift  $\phi_{0l}$  defined by (26) we may formulate the expression of the wave function for a stationary state with one bound pair, omitting an irrelevant overall phase

factor:

$$\begin{aligned}
\Omega_{k,r,m} &= \sum_{l=1}^{r-1} \sum_{1 \leq j_1 < j_2 < \dots < j_{l-1} < n_0 < j_{l+2} - 1 < j_{l-1} - 1 < \dots < j_r - 1 \leq N-1} \sum \\
&e^{-i\pi n_0} \sum_P \prod_{p < l} e^{-i\phi_{0p}} \prod_{l=3}^r e^{ik_{P(l)} j_l} \times \\
&\times \sum_{q < t, Pq > P(t)} e^{i\phi_{P(q)P(t)}} \Phi_{j_1 j_2 \dots j_{l-1} n_0 j_{l+2} \dots j_r} + \\
&+ \sum_{2 \leq j_3 < j_4 < \dots < j_{r-2} < n_0 = N} \\
&\sum_P e^{-i\pi N} \prod_{p=3}^{r-2} e^{-i\phi_{0p}} \prod_{l=3}^r e^{ik_{P(l)} j_l} \times \\
&\times \sum_{q < t, Pq > P(t)} e^{i\phi_{P(q)P(t)}} \Phi_{j_3 j_4 \dots j_{r-2} n_0 = N}.
\end{aligned} \tag{27}$$

Again we will identify the 2 representations of a stationary state in this case: On the one hand the representation given by (4) and on the other hand (27), translated in terms of the parameters  $x_p (p = 3, 4, \dots, r)$ . The product of an ESP of the parameters and a coefficient in  $\Omega_{k,r,m}$  corresponding with given distances between the deviations again results in a linear combination of coefficients, which enables us to find linear equations for the ESP. This will be illustrated by some examples in section 6.

### 5. Examples 1. States without a bound pair

Formula (18) will now be used to derive linear equations for the ESP with coefficients given by the amplitudes in the standard representation.

We may restrict ourselves to the cases  $N = 2r$  ( $N$  even) or  $N = 2r + 1$  ( $N$  odd). The case  $r = 1$  will not be considered because it represents an unperturbed plane wave.

#### 5.1. $r = 2, N = 4, 5$

There are 2 quantities in this case  $k$  and  $E$ , where  $E$  is the energy of the eigenstates of the Heisenberg Hamiltonian. They completely determine the solution, so further analysis is not necessary, if these two are known. But as a simple illustration of our analysis we write (18) for  $r = 2$ :

$$\begin{aligned}
&c(d_1, (N - d_1)) \\
&= \sum_P x_{P(2)}^{d_1} \prod_{P(2) < P(1)} \left( \frac{2x_{P(1)} - x_{P(1)}x_{P(2)} - 1}{2x_{P(2)} - x_{P(1)}x_{P(2)} - 1} \right) \\
&= x_2^{d_1} - x_1^{d_1} \frac{2x_2 - x_1x_2 - 1}{2x_1 - x_1x_2 - 1}, \quad d_1 = 1, 2.
\end{aligned} \tag{28}$$

From this equation we derive in an easy way:

$$\begin{aligned}
A_1 c(1, (N - 1)) &= -x_1 x_2 c(0, (N)) - c(2, (N - 2)) \\
&= -A_2 c(0, (N)) - c(2, (N - 2)) \\
A_1 c(2, (N - 2)) &= -x_1 x_2 c(1, (N - 1)) - c(3, (N - 3)) \\
&= -A_2 c(1, (N - 1)) - c(3, (N - 3)).
\end{aligned} \tag{29}$$

The last one of these equations gives for  $N = 4, 5$  respectively:

$$N = 4 : A_1 c(2, (2)) + (e^{ik} + e^{3ik}) c(1, (3)) = 0 \quad (30)$$

$$N = 5 : (A_1 + e^{3ik}) c(2, (3)) + e^{ik} c(1, (4)) = 0. \quad (31)$$

These equations give the correct  $A_1$  and  $A_2$  for given amplitudes  $c(d_1, (N - d_1))$  with the exception of the case ( $N = 4, c(2, (2)) = 0$ ), representing a state with a bound pair, for which we find the following values of the parameters:

$$\begin{aligned} k &= -\pi \text{ or } A_2 = -1 \\ c(2, (2)) &= 0 \end{aligned} \quad (32)$$

which according to (30) should result in  $c(1, (3)) = 0$ , which means no solution. Formally we could construct a solution of (32) and (30) for which  $A_1 = \infty$ , but we prefer the description in terms of the modified B.H. scheme, analyzed in section 4.

### 5.2. $r = 3, N = 6, 7$

For a given solution in the standard form we know the parameter set  $(k, E)$ , so we need one further equation to determine completely the B.H.-parameters in terms of the amplitudes  $c(d_1, d_2, (N - d_1 - d_2))$ . Formula (18) now takes the form:

$$c(d_1, d_2, (N - d_1 - d_2)) = \sum_P x_{P(2)}^{d_1} x_{P(3)}^{d_1+d_2} \prod_{\substack{1 \leq l < p \leq 3 \\ P(l) > P(p)}} \left( -\frac{2x_{P(l)} - x_{P(l)}x_{P(p)} - 1}{2x_{P(p)} - x_{P(l)}x_{P(p)} - 1} \right) \quad (33)$$

from which we derive:

$$\begin{aligned} &A_1 c(d_1, d_2, (N - d_1 - d_2)) \\ &= -e^{ik} c(d_1 - 1, d_2, (N + 1 - d_1 - d_2)) - c(d_1 + 1, d_2 - 1, (N - d_1 - d_2)) + \\ &\quad - c(d_1, d_2 + 1, (N - 1 - d_1 - d_2)) \end{aligned} \quad (34)$$

$$\begin{aligned} &A_2 c(d_1, d_2, (N - d_1 - d_2)) \\ &= e^{ik} [c(d_1, d_2 - 1, (N + 1 - d_1 - d_2)) + c(d_1 - 1, d_2 + 1, (N - d_1 - d_2))] + \\ &\quad + c(d_1 + 1, d_2, (N - 1 - d_1 - d_2)) \end{aligned} \quad (35)$$

with:

$$A_1 = -(x_1 + x_2 + x_3) \quad A_2 = x_1 x_2 + x_1 x_3 + x_2 x_3. \quad (36)$$

For  $N = 7$  (34) and (35) give us 2 equations for  $A_1$  and  $A_2$  taking  $d_1 = d_2 = 2$ . These equations contain as coefficients the amplitudes  $c$  without an entry 0. The coefficient of  $A_1$  and  $A_2$  in these equations:  $c(2, 2, (3))$ , is supposed to be unequal to 0. (N.B.: If this should be the case a modification of the procedure given for  $N = 6$  will result in an alternative set of equations).

For  $N = 6$  the situation is more interesting. First of all we may write down the equations for  $d_1 = d_2 = 2$ , making use of the periodic boundary conditions expressed by (10):

$$\begin{aligned} A_1 c(2, 2, (2)) &= -(e^{ik} + e^{3ik} + e^{5ik}) c(1, 2, (3)) \\ A_2 c(2, 2, (2)) &= (e^{ik} + e^{3ik} + e^{5ik}) c(1, 3, (2)). \end{aligned} \quad (37)$$

These equations give us the ESP  $A_1$  and  $A_2$  in terms of the coefficients  $c$ , again with the exception of the case for which  $c(2, 2, (2)) = 0$ , i.e. for  $k = \mp\pi/3$  and  $\mp 2\pi/3$ . In that case we

have to make use of other values of  $d_1$  and  $d_2$  and the result will be a set of equations that contain coefficients  $c$  with one entry 0. These coefficients should be eliminated and the only possibility is that there appears only *one* such a coefficient in the eq. (34) and (35) and it should be the same in both equations. This may be realized with the following combination:

$$\begin{aligned} A_1 c(1, 3, (2)) &= -e^{5ik} c(1, 1, (4)) - e^{ik} c(0, 3, (3)) \\ A_2 c(1, 2, (3)) &= e^{ik} c(1, 1, (4)) + e^{ik} c(0, 3, (3)) \end{aligned} \quad (38)$$

which add up to:

$$A_1 c(1, 3, (2)) + A_2 c(1, 2, (3)) = (e^{ik} - e^{5ik}) c(1, 1, (4)) \quad (39)$$

which cover all the possible cases for which  $c(2, 2, (2)) = 0$ , again with the exception of the states with a bound pair, discussed in the section 4.

### 5.3. $r = 4, N = 8, 9$

Here we focus on the interesting case  $N = 8$ , for which we have the ESP:

$$\begin{aligned} A_1 &= -(x_1 + x_2 + x_3 + x_4) \quad A_2 = x_1 x_2 + x_1 x_3 + x_1 x_4 + x_2 x_3 + x_2 x_4 + x_3 x_4 \\ A_3 &= -(x_1 x_2 x_3 + x_1 x_2 x_4 + x_1 x_3 x_4 + x_2 x_3 x_4). \end{aligned} \quad (40)$$

Apart from the quantities  $(k, E)$  we need two other relations between the  $x_l (l = 1, \dots, 4)$  to determine completely the the solution.

For this case we may derive from (18) for  $r = 4$ :

$$\begin{aligned} &A_1 c(d_1, d_2, d_3, (8 - d_1 - d_2 - d_3)) \\ &= -e^{ik} c(d_1 - 1, d_2, d_3, (9 - d_1 - d_2 - d_3)) - \\ &\quad -c(d_1 + 1, d_2 - 1, d_3, (8 - d_1 - d_2 - d_3)) + \\ &\quad -c(d_1, d_2 + 1, d_3 - 1, (8 - d_1 - d_2 - d_3)) + \\ &\quad -c(d_1, d_2, d_3 + 1, (7 - d_1 - d_2 - d_3)) \end{aligned} \quad (41)$$

$$\begin{aligned} &A_2 c(d_1, d_2, d_3, (8 - d_1 - d_2 - d_3)) \\ &= e^{ik} [c(d_1, d_2 - 1, d_3, (9 - d_1 - d_2 - d_3)) + \\ &\quad +c(d_1 - 1, d_2 + 1, d_3 - 1, (9 - d_1 - d_2 - d_3)) + \\ &\quad +c(d_1 - 1, d_2, d_3 + 1, (8 - d_1 - d_2 - d_3))] + \\ &\quad +c(d_1 + 1, d_2, d_3 - 1, (8 - d_1 - d_2 - d_3)) + \\ &\quad +c(d_1 + 1, d_2 - 1, d_3 + 1, (7 - d_1 - d_2 - d_3)) + \\ &\quad +c(d_1, d_2 + 1, d_3, (7 - d_1 - d_2 - d_3)) \end{aligned} \quad (42)$$

$$\begin{aligned} &A_3 c(d_1, d_2, d_3, (8 - d_1 - d_2 - d_3)) \\ &= -e^{ik} [c(d_1, d_2, d_3 - 1, (9 - d_1 - d_2 - d_3)) + \\ &\quad +c(d_1, d_2 - 1, d_3 + 1, (8 - d_1 - d_2 - d_3)) + \\ &\quad +c(d_1 - 1, d_2 + 1, d_3, (8 - d_1 - d_2 - d_3))] + \\ &\quad -c(d_1 + 1, d_2, d_3, (7 - d_1 - d_2 - d_3)) \end{aligned} \quad (43)$$



from which it follows, again taking into account proper boundary conditions:

$$\begin{aligned}
A_1 c(2, 2, 2, (2)) &= -(e^{ik} + e^{3ik} + e^{5ik} + e^{7ik})c(1, 2, 2, (3)) \\
A_2 c(2, 2, 2, (2)) &= (e^{ik} + e^{3ik} + e^{5ik} + e^{7ik})c(1, 2, 3, (2)) + \\
&\quad + (e^{ik} + e^{3ik})c(1, 3, 1, (3)) \\
A_3 c(2, 2, 2, (2)) &= -(e^{ik} + e^{3ik} + e^{5ik} + e^{7ik})c(1, 3, 2, (2))
\end{aligned} \tag{44}$$

from which we may derive the ESP, again with one possible exception, i.e.:  $c(2, 2, 2, (2)) = 0$ . For  $c(2, 2, 2, (2)) \neq 0$  we may choose two of the equations (44) to find all  $A_n (n = 1, \dots, 4)$  and consequently all  $x_j (j = 1, \dots, 4)$ .

For the other possibility we need two additional equations derived from (41-43). We first look for a coefficient  $c$  with one entry 0 that is generated at least two times, so that it may be eliminated. The simplest example that we could find is:

$$c(0, 3, 2, (3)) \tag{45}$$

that is generated in 2 ways:

$$\begin{aligned}
&A_1 c(1, 3, 2, (2)) \\
&= -e^{ik} c(0, 3, 2, (3)) - c(1, 4, 1, (2)) - c(1, 3, 3, (1)) \\
&A_3 c(1, 2, 2, (3)) \\
&= -e^{ik} [c(1, 2, 1, (4)) + c(1, 1, 3, (3)) + c(0, 3, 2, (3))]
\end{aligned} \tag{46}$$

from which it immediately follows:

$$\begin{aligned}
&A_1 c(1, 3, 2, (2)) - A_3 c(1, 2, 2, (3)) \\
&= (e^{ik} - e^{7ik})c(1, 1, 3, (3)) + (e^{ik} - e^{5ik})c(1, 2, 1, (4)).
\end{aligned} \tag{47}$$

The next example is:

$$c(0, 2, 3, (3)) \tag{48}$$

which is generated again in two ways:

$$\begin{aligned}
A_1 c(1, 2, 3, (2)) &= -e^{7ik} c(1, 1, 2, (4)) - (1 + e^{2ik})c(1, 3, 2, (2)) - e^{ik} c(0, 2, 3, (3)) \\
A_2 c(1, 2, 2, (3)) &= e^{ik} c(1, 1, 2, (4)) + (1 + e^{2ik} + e^{4ik})c(1, 3, 2, (2)) + \\
&\quad + e^{ik} [c(0, 2, 3, (3)) + c(0, 3, 1, (4))].
\end{aligned} \tag{49}$$

But this introduces another non-vanishing amplitude with an entry 0:

$$c(0, 3, 1, (4)) \tag{50}$$

which in its turn also appears in:

$$A_1 c(1, 3, 1, (3)) = -(1 + e^{4ik})c(1, 3, 2, (2)) - (e^{ik} + e^{5ik})c(0, 3, 1, (4)). \tag{51}$$

Now a proper linear combination of the two equations (49) and (51) gives:

$$\begin{aligned}
&A_1 [(e^{ik} + e^{5ik})c(1, 2, 3, (2)) + e^{ik} c(1, 3, 1, (3))] + A_2 (e^{ik} + e^{5ik})c(1, 2, 2, (3)) \\
&= -(1 - e^{2ik} + e^{4ik} - e^{6ik})c(1, 1, 2, (4)).
\end{aligned} \tag{52}$$

In a completely analogous way we find the equation:

$$\begin{aligned} & A_2(e^{ik} + e^{5ik})c(1, 3, 2, (2)) + A_3[(e^{ik} + e^{5ik})c(1, 2, 3, (2)) + e^{ik}c(1, 3, 1, (3))] \\ = & (1 - e^{2ik} + e^{4ik} - e^{6ik})c(1, 1, 4, (2)). \end{aligned} \quad (53)$$

In the last example we consider:

$$c(0, 4, 2, (2)) \quad (54)$$

which is generated in the two equations:

$$\begin{aligned} & A_1c(1, 1, 4, (2)) \\ = & -e^{7ik}c(1, 1, 1, (5)) - c(1, 2, 3, (2)) - e^{ik}c(0, 1, 4, (3)) - e^{2ik}c(0, 4, 2, (2)) \\ & A_2c(1, 1, 3, (3)) \\ = & (1 + e^{2ik})c(1, 2, 3, (2)) + \\ & e^{ik}c(0, 1, 4, (3)) + e^{ik}c(0, 2, 2, (4)) + e^{2ik}c(0, 3, 4, (1)) + e^{2ik}c(0, 4, 2, (2)). \end{aligned} \quad (55)$$

Now we have to look for a second way to generate:

$$c(0, 2, 2, (4)) \quad (56)$$

which is:

$$\begin{aligned} & A_3c(1, 1, 2, (4)) \\ = & -e^{ik}c(1, 1, 1, (5)) - e^{2ik}c(1, 2, 3, (2)) + \\ & -e^{ik}c(0, 2, 2, (4)) - e^{2ik}c(0, 3, 4, (1)) \end{aligned} \quad (57)$$

and it turns out that we may find a linear combination of the 2 equations of (55) together with (57) for which the amplitudes (54) and (56) as well as:

$$c(0, 1, 4, (3)) \quad \text{and} \quad c(0, 3, 4, (1)) \quad (58)$$

disappear. This combination is:

$$A_1c(1, 1, 4, (2)) + A_2c(1, 1, 3, (3)) + A_3c(1, 1, 2, (4)) = -(e^{ik} + e^{7ik})c(1, 1, 1, (5)). \quad (59)$$

N.B.1: As was stated before for the case ( $N = 8, r = 4$ ) with  $c(2, 2, 2, (2)) = 0$  we only need *two* additional equations to determine the complete set of ESP. We may choose two from the set (47),(52),(53),(59).

N.B. 2: Also in this case the states with a bound pair should be analyzed according to the method of the next section.

General remark: We have not given explicit numeral examples of our analysis, but our method could be easily checked, also for its completeness, with the results we have for  $N = 4, 6$  and  $8$  in other papers.

## 6. Examples 2. States with one bound pair

In this section we only consider 2 simple examples, i.e. *one* bound pair in combination with one or two "free" deviations, respectively corresponding with  $r = 3$  and  $r = 4$ . For these cases we do not need the ESP to determine the wave numbers of these free deviations:  $k_3$  ( $r = 3$ ) and the pair  $(k_3, k_4)$  ( $r = 4$ ).

### 6.1. $r = 3$

The state vector has the following form for this case, according to section 4:

$$\begin{aligned} \Omega_{k,3,m} &= \sum_{1 \leq n_0 < j_3 - 1 \leq N-1} e^{-i\pi n_0} e^{ik_3 j_3} \Phi_{n_0 j_3} + \\ &+ e^{-i\phi_{03}} \sum_{2 \leq j_3 < n_0 \leq N} e^{-i\pi n_0} e^{ik_3 j_3} \Phi_{j_3 n_0} \end{aligned} \quad (60)$$

$$e^{i\phi_{03}} = \frac{2 - x_3}{x_3(2x_3 - 1)} \quad x_3 = e^{ik_3}. \quad (61)$$

N.B.: The term  $\Phi_{j_3 n_0 = N}$  represents a state with a bound pair on the sites  $(N, N+1) \equiv (1, N)$ .

Periodic boundary conditions are now formulated in the following way. We take a term in the first sum with an index  $j_3$  outside the prescribed range and identify this term with one in the second sum:

$$j_3 \Rightarrow j'_3 + N, \quad j'_3 < n_0$$

and a term in the second summation with:  $n_0 \Rightarrow n'_0 + N, n'_0 < j_3 - 1$ , which may be identified with a term of the first summation:

$$n_0 \Rightarrow n'_0 + N, \quad n'_0 < j_3 - 1.$$

This results in 2 boundary conditions:

$$x_3^N = \frac{x_3(2x_3 - 1)}{2 - x_3} \quad (62)$$

and:

$$\frac{x_3(2x_3 - 1)}{2 - x_3} e^{-i\pi N} = 1 \quad (63)$$

For even  $N$  this results in the equation:

$$x_3^N = \frac{x_3(2x_3 - 1)}{2 - x_3} = 1 \quad (64)$$

and for odd  $N$ :

$$x_3^N = \frac{x_3(2x_3 - 1)}{2 - x_3} = -1 \quad (65)$$

For the first case,  $N$  is even, (64) gives an acceptable solution:

$$x_3 = \mp 1 \quad (66)$$

For odd values of  $N$  (65) gives a solution:

$$x_3 = e^{\mp i\pi/3} \quad N = 3, 9, 15, \dots \quad (67)$$

6.2.  $r = 4$  :

The state vector for this case according to section 4, takes the form:

$$\begin{aligned}
\Omega_{k,4,m} = & \sum_{1 \leq n_0 < j_3 - 1 < j_4 - 1 \leq N-1} e^{-i\pi n_0} [e^{i(k_3 j_3 + k_4 j_4)} + \\
& + e^{i\phi_{43}} e^{i(k_4 j_3 + k_3 j_4)}] \Phi_{n_0 j_3 j_4} + \\
& + \sum_{1 \leq j_3 < n_0 < j_4 - 1 \leq N-1} e^{-i\pi n_0} [e^{-i\phi_{03}} e^{i(k_3 j_3 + k_4 j_4)} + \\
& + e^{i\phi_{43}} e^{-i\phi_{04}} e^{i(k_4 j_3 + k_3 j_4)}] \Phi_{j_3 n_0 j_4} + \\
& + \sum_{1 \leq j_3 < j_4 < n_0 \leq N} e^{-i\pi n_0} e^{-i(\phi_{03} + \phi_{04})} [e^{i(k_3 j_3 + k_4 j_4)} + \\
& + e^{i\phi_{43}} e^{i(k_4 j_3 + k_3 j_4)}] \Phi_{j_3 j_4 n_0}
\end{aligned} \tag{68}$$

In the first summation we now take the following index values, for  $j_4$  outside the prescribed range:

$$j_4 \Rightarrow j'_3 + N, j'_3 < n_0, j_3 \Rightarrow j'_4$$

and find the following term:

$$e^{-i\pi n_0} [e^{ik_3 N} e^{i\phi_{43}} e^{i(k_3 j'_3 + k_4 j'_4)} + e^{ik_4 N} e^{i(k_4 j'_3 + k_3 j'_4)}] \Phi_{j'_3 n_0 j'_4}. \tag{69}$$

In the second summation we take:

$$j_4 \Rightarrow j'_3 + N, j_3 \Rightarrow j'_4, j'_4 < n_0$$

which results in :

$$e^{-i\pi n_0} [e^{-i\phi_{04}} e^{ik_3 N} e^{i\phi_{43}} e^{i(k_3 j'_3 + k_4 j'_4)} + e^{-i\phi_{03}} e^{ik_4 N} e^{i(k_4 j'_3 + k_3 j'_4)}] \Phi_{j'_3 j'_4 n_0} \tag{70}$$

and finally in the third summation:

$$n_0 \Rightarrow n'_0 + N, j_3 \Rightarrow j'_3, j_4 \Rightarrow j'_4$$

which gives:

$$e^{-i\pi n_0} e^{-i\pi N} e^{-i(\phi_{03} + \phi_{04})} [e^{i(k_3 j'_3 + k_4 j'_4)} + e^{i\phi_{43}} e^{i(k_4 j'_3 + k_3 j'_4)}] \Phi_{n_0 j'_3 j'_4}. \tag{71}$$

Now we identify (69) with a term in the second summation in (68) , (70) with a term in the third summation and (71) with one in the first summation, which gives the following three equations:

$$\begin{aligned}
e^{ik_3 N} e^{i\phi_{43}} &= e^{-i\phi_{03}} e^{ik_4 N} = e^{i\phi_{43}} e^{-i\phi_{04}} \\
e^{-i\pi N} e^{-i(\phi_{03} + \phi_{04})} &= 1
\end{aligned} \tag{72}$$

For even  $N$  the translation into the variables  $x_3$  and  $x_4$  read:

$$\begin{aligned}
x_3^N \frac{2x_4 - x_3 x_4 - 1}{2x_3 - x_3 x_4 - 1} \frac{2 - x_3}{x_3(2x_3 - 1)} &= -1 \\
x_4^N \frac{2x_3 - x_3 x_4 - 1}{2x_4 - x_3 x_4 - 1} \frac{2 - x_4}{x_4(2x_4 - 1)} &= -1 \\
\frac{2 - x_3}{x_3(2x_3 - 1)} \frac{2 - x_4}{x_4(2x_4 - 1)} &= 1
\end{aligned} \tag{73}$$

from which it follows in an easy way:

$$(x_3x_4)^N = 1 \quad (74)$$

consistent with the periodic boundary conditions as a consequence of the fact that the total wave number should obey:

$$k = -\pi + k_3 + k_4 = 2\pi\lambda/N, \quad \lambda = -N/2, -N/2 + 1, \dots, N/2 - 1. \quad (75)$$

The last equation of (73) implies:

$$(1 - x_3x_4)[2(1 + x_3x_4) - (x_3 + x_4)] = 0 \quad (76)$$

which results in either one of the following possibilities:

$$\begin{aligned} x_3x_4 &= 1 \\ x_3 + x_4 &= 2(1 + x_3x_4) \end{aligned} \quad (77)$$

The wave numbers corresponding with  $x_3$  and  $x_4$  should be complex conjugated because of (75):

$$k_3 = \text{Re}(k_3) - i\delta \quad k_4 = \text{Re}(k_3) + i\delta \quad \delta \text{ is real} \quad (78)$$

The only acceptable solutions of (76) turn out to be:

$$\begin{aligned} x_3x_4 &= 1 \quad k_3 = -k_4 \quad k = -\pi \\ x_3x_4 &= -1 \quad x_3 = -x_4 = \pm 1 \end{aligned} \quad (79)$$

The second equation results in:

$$k = 0 : K_0 = -\pi, k_3 = 0, k_4 = \pi \quad (80)$$

whereas the first one, together with the first equation of (73), results in a series of solutions given by:

$$x_3^{N-2}(2 - x_3) - (2x_3 - 1) = 0 \quad (81)$$

For the case  $N = 8$  this equation takes the form:

$$x_3^7 - 2x_3^6 + 2x_3 - 1 = 0 \quad (82)$$

with solutions:

$$k_3 = (0, \mp 2.5864, \mp 1.4509, \mp i0.66662) \quad (83)$$

These results were already published in an earlier paper [4].

N.B.: In general one may treat the parts of the wave function (68) representing the individual wavelike deviations for a given position of the coupled pair, in the same way as the state vector for a solution without a bound pair, i.e. from these parts we may derive again a set of equations for the ESP of the  $x_l$  of all the deviations apart from those of the coupled pair.

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