Quantum numbers for relative ground states of antiferromagnetic Heisenberg spin rings

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(Dated: June 5, 2003)

We suggest a general rule for the shift quantum numbers k of the relative ground states of antiferromagnetic Heisenberg spin rings. This rule generalizes well-known results of Marshall, Peierls, Lieb, Schultz, and Mattis for even rings. Our rule is confirmed by numerical investigations and rigorous proofs for special cases, including systems with a Haldane gap for $N \to \infty$. Implications for the total spin quantum number S of relative ground states are discussed as well as generalizations to the XXZ model.

PACS numbers: 75.10.-b,75.10.Jm,75.50.Ee

Keywords: Molecular magnets, Heisenberg model, spin rings, antiferromagnetism

I. INTRODUCTION

Rigorous results on spin systems like the Marshall-Peierls sign rule[1] and the famous theorems of Lieb, Schultz, and Mattis[2,3] have sharpened our understanding of magnetic phenomena. They also serve as a theoretical input for quantum computing with spin systems.[4–6]

Exact diagonalization methods yield the energy eigenvalues and eigenvectors for small spin rings of various numbers N of spin sites and spin quantum numbers s where the interaction is given by antiferromagnetic nearest neighbor exchange[7–12]. One quantity of interest is the shift quantum number $k = 0, \dots N-1$ associated with the cyclic shift symmetry of the rings. The corresponding crystal momentum is then $2\pi k/N$. Using the sign rule of Marshall and Peierls[1] or equivalently the theorems of Lieb, Schultz, and Mattis[2,3] one can explain the shift quantum numbers for the relative ground states in subspaces $\mathcal{H}(M)$ of total magnetic quantum number M for rings with even N. In the case of single-spin quantum number $s = 1/2$ one knows the shift quantum numbers of the total ground states for all N via the Bethe ansatz.[10]

The sign rule of Marshall and Peierls as well as the theorems of Lieb, Schultz, and Mattis only apply to bipartite rings, i. e. rings with even N. Nevertheless, even for frustrated rings with odd N astonishing regularities are numerically verified. This creates the need for a deeper insight or – at best – an analytic proof for the simple k-rule 1 (see below) which comprises all these results. Unifying the picture for even and odd N, we find for the ground state without exception:[11,12]

1. The ground state belongs to the subspace $\mathcal{H}(S)$ with the smallest possible total spin quantum number S; this is either $S = 0$ for $N{\cdot}s$ integer, then the total magnetic quantum number M is also zero, or $S = 1/2$ for $N \cdot s$ half integer, then $M = \pm 1/2$.
2. If $N \cdot s$ is integer, then the ground state is non-degenerate.
3. If $N{\cdot}s$ is half integer, then the ground state is four-fold degenerate.
4. If s is integer or $N{\cdot}s$ even, then the shift quantum number is $k = 0$.
5. If s is half integer and $N \cdot s$ odd, then the shift quantum number turns out to be $k = N/2$.
6. If $N{\cdot}s$ is half integer, then $k = \lfloor (N+1)/4 \rfloor$ and $k = N - \lfloor (N+1)/4 \rfloor$ is found. $\lfloor (N+1)/4 \rfloor$ symbolizes the greatest integer less than or equal to $(N+1)/4$.

N	s	a										
		1	2	3	4	5	6	7	8	9	10	11
3	1/2	1,2	-	-	-	-	-	-	-	-	-	-
3	1	1,2	**0**,1,2	0	-	-	-	-	-	-	-	-
3	3/2	1,2	**0**,1,2	0,**1**,**2**	1,2	-	-	-	-	-	-	-
3	2	1,2	**0**,1,2	0,**1**,**2**	**0**,1,2	**0**,1,2	0	-	-	-	-	-
5	1/2	2,3	1,4	-	-	-	-	-	-	-	-	-
5	1	2,3	1,4	1,4	2,3	0	-	-	-	-	-	-
5	3/2	2,3	1,4	1,4	2,3	0	2,3	1,4	-	-	-	-
5	2	2,3	1,4	1,4	2,3	0	2,3	1,4	1,4	2,3	0	-
7	1/2	3,4	1,6	2,5	-	-	-	-	-	-	-	-
7	1	3,4	1,6	2,5	2,5	1,6	3,4	0	-	-	-	-
7	3/2	3,4	1,6	2,5	2,5	1,6	3,4	0	3,4	1,6	2,5	-
9	1/2	4,5	1,8	3,6	2,7	-	-	-	-	-	-	-
9	1	4,5	1,8	3,6	2,7	2,7	3,6	1,8	4,5	0	-	-
11	1/2	5,6	1,10	4,7	2,9	3,8	-	-	-	-	-	-
11	1	5,6	1,10	4,7	2,9	3,8	3,8	2,9	4,7	1,10	5,6	0

TABLE I: Numerically verified shift quantum numbers for selected N and s in subspaces $\mathcal{H}(M)$. Instead of M the quantity $a = Ns - M$ is used. The shift quantum number for the magnon vacuum $a = 0$ is always $k = 0$. The shift quantum numbers are invariant under $a \leftrightarrow 2Ns - a$ and hence only displayed for $a = 1, 2, \dots, \lfloor Ns \rfloor$. Extraordinary shift quantum numbers given in bold do not comply with Eq. 1.

In this article we will extend the knowledge about shift quantum numbers to the relative ground states in subspaces $\mathcal{H}(M)$ for odd rings. Table I shows a small selection of shift quantum numbers for some N and s. The dependence of k on N and M or, equivalently, on N and the magnon number $a = Ns - M$ can – for even as well as for odd N – be generalized as given by the following

k-rule 1

$$\textit{If}\, N \neq 3 \quad \textit{then} \quad k \equiv \pm a \lceil \frac{N}{2} \rceil \mod N \ . \qquad (1)$$

Moreover the degeneracy of the relative ground state is minimal.

Here $\lceil N/2 \rceil$ denotes the smallest integer greater than or equal to $N/2$. "Minimal degeneracy" means that the relative ground state in $\mathcal{H}(M)$ is twofold degenerate if there are two different shift quantum numbers and non-degenerate if $k = 0 \mod N$ or $k = N/2 \mod N$, the latter for even N.

It is noteworthy that the shift quantum numbers do not explicitely depend on s. For $N = 3$ and $3s - 2 \geq |M| \geq 1$ we find besides the ordinary shift quantum numbers given by (1) extraordinary shift quantum numbers, which supplement the ordinary ones to the complete set $\{k\} = \{0, 1, 2\}$. This means an additional degeneracy of the respective relative ground state, which is caused by the high symmetry of the Heisenberg triangle.

For even N the k-rule (1) results in an alternating k-sequence $0, N/2, 0, N/2, \ldots$ on descending from the magnon vacuum with $M = Ns$, i. e. $a = 0$, which immediately implies that the ground state in $\mathcal{H}(M)$ has the total spin quantum number $S = |M|$, compare Refs. 1–3.

For odd N the regularity following from (1) will be illustrated by an example: Let $N = 11$ and s be sufficiently large. Then the k-sequence reads $0, \pm 6, \pm 1, \pm 7, \pm 2, \pm 8, \pm 3, \pm 9, \pm 4, \pm 10, \pm 5, 0, \ldots$, where all shift quantum numbers are understood mod 11. The sequence is periodic with period 11 and repeats itself after 5 steps in reverse order. In the first 5 steps each possible k-value is assumed exactly once. Since $\pm 8 = \mp 3$ mod 11, the shift quantum numbers for $a = 5$ and $a = 6$ are the same, likewise for $a = 16$ and $a = 17$ and so on.

The last finding can be easily generalized: For odd N the k quantum numbers are the same in adjacent subspaces $\mathcal{H}(M = Ns - a)$ and $\mathcal{H}(M' = Ns - (a+1))$ iff N divides $(2a + 1)$. In such cases one cannot conclude that the ground state in $\mathcal{H}(M)$ has the total spin quantum number $S = |M|$, nevertheless, in all other cases including the total ground state one can, see section III.

The k-rule 1 is founded in a mathematically rigorous way for N even,[1–3] $N = 3$ (including extraordinary k numbers, see section IV C), $a = 0$ (trivial), $a = 1$ (cf. section IV A), $a = 2$ (but only in a weakened version, cf. section IV D). For the ground state with N odd, $s = 1/2$ the k-rule follows from the Bethe ansatz, cf. section IV B. An asymptotic proof for large enough N is provided in section IV E for systems with an asymptotically finite excitation gap (Haldane systems). The k-rule also holds for the exactly solvable XY-model with $s = 1/2$, cf. section VI. For $N{\cdot}s$ being half integer field theory methods yield that the ground state shift quantum number approaches $N/4$ for large N.[13] Apart from these findings a rigorous proof of the k-rule still remains a challenge.

II. HEISENBERG MODEL

The Hamilton operator of the Heisenberg model with antiferromagnetic, isotropic nearest neighbor interaction between spins of equal spin quantum number s is given by

$$\underset{\sim}{H} \ \equiv \ 2 \sum_{i=1}^{N} \underset{\sim}{\vec{s}}_i \cdot \underset{\sim}{\vec{s}}_{i+1} \ , \quad N+1 \equiv 1 \ . \qquad (2)$$

$\underset{\sim}{H}$ is invariant under cyclic shifts generated by the shift operator $\underset{\sim}{T}$. $\underset{\sim}{T}$ is defined by its action on the product basis $|\, \vec{m}\, \rangle$

$$\underset{\sim}{T} \ |\, m_1, \ldots, m_N \,\rangle \equiv |\, m_N, m_1, \ldots, m_{N-1} \,\rangle \ , \qquad (3)$$

where the product basis is constructed from single-particle eigenstates of all $\underset{\sim}{s}_i^3$

$$\underset{\sim}{s}_i^3 \ |\, m_1, \ldots, m_N \,\rangle = m_i \ |\, m_1, \ldots, m_N \,\rangle \ . \qquad (4)$$

The shift quantum number $k = 0, \ldots, N-1$ modulo N labels the eigenvalues of $\underset{\sim}{T}$ which are the N-th roots of unity

$$z = \exp\left\{ -i \frac{2\pi k}{N} \right\} \ . \qquad (5)$$

Altogether $\underset{\sim}{H}$, $\underset{\sim}{T}$, the square $\underset{\sim}{\vec{S}}^2$, and the three-component $\underset{\sim}{S}^3$ of the total spin are four commuting operators. The subspaces of states with the quantum numbers M, S, k will be denoted by $\mathcal{H}_N(M, S, k)$.

The Hamilton operator (2) can be cast in the form

$$\underset{\sim}{H} \ = \ \underset{\sim}{\Delta} + \underset{\sim}{G} + \underset{\sim}{G}^\dagger \ , \qquad (6)$$

where we introduced

$$\underset{\sim}{\Delta} \ \equiv \ 2 \sum_{i=1}^{N} \underset{\sim}{s}_i^3 \underset{\sim}{s}_{i+1}^3 \ , \qquad (7)$$

and the "generation operator"

$$\underset{\sim}{G} \ \equiv \ \sum_{i=1}^{N} \underset{\sim}{s}_i^- \underset{\sim}{s}_{i+1}^+ \qquad (8)$$

together with its adjoint $\underset{\sim}{G}^\dagger$.

It follows that $\underset{\sim}{H}$ is represented by a real matrix with respect to the product basis. Hence if an eigenvector of this matrix has the shift quantum number k, its complex conjugate will be again an eigenvector with the same eigenvalue but with shift quantum number $-k \mod N$. Simultaneous eigenvectors of $\underset{\sim}{H}$ and $\underset{\sim}{T}$ can be chosen to be real in the product basis only if $k = 0$ or $k = N/2$.

We define a unitary "Bloch" operator $\underset{\sim}{U}$ for spin rings, compare Refs. 2,14,

$$\underset{\sim}{U} \equiv \exp\left\{ \frac{2\pi i}{N} \sum_{j=1}^{N} j\,(s - \underset{\sim}{s}_j^3) \right\} , \tag{9}$$

which is diagonal in the product basis (4).

We then have, with a little bit of calculation,

$$\underset{\sim}{T}\underset{\sim}{U}\underset{\sim}{T}^\dagger\underset{\sim}{U}^\dagger = \exp\left\{ -\frac{2\pi i}{N} \sum_{j=1}^{N} (s - \underset{\sim}{s}_j^3) \right\} \tag{10}$$

$$= \exp\left\{ -\frac{2\pi i}{N}\, a \right\} , \tag{11}$$

where the last line (11) holds in subspaces $\mathcal{H}(M = Ns - a)$. Consequently, $\underset{\sim}{U}$ is a shift operator in k-space and shifts the quantum number k of a state $|\,\phi\,\rangle \in \mathcal{H}(M)$ by a:

$$\text{If } \underset{\sim}{T}\,|\,\phi\,\rangle = \exp\left\{ -\frac{2\pi i}{N}\, k \right\} |\,\phi\,\rangle \tag{12}$$

$$\text{then } \underset{\sim}{T}\underset{\sim}{U}\,|\,\phi\,\rangle = \exp\left\{ -\frac{2\pi i}{N}\,(k+a) \right\} \underset{\sim}{U}\,|\,\phi\,\rangle .$$

We also observe that

$$\underset{\sim}{U}\underset{\sim}{G}\underset{\sim}{U}^\dagger = \exp\left\{ -\frac{2\pi i}{N} \right\} \underset{\sim}{G} , \tag{13}$$

and define the unitary "Bloch" transform of the Hamilton operator

$$\widehat{\underset{\sim}{H}}(\ell) \equiv \underset{\sim}{U}^\ell \underset{\sim}{H} (\underset{\sim}{U}^\dagger)^\ell = \underset{\sim}{\Delta} + \cos\left(\frac{2\pi\ell}{N}\right) \left\{ \underset{\sim}{G} + \underset{\sim}{G}^\dagger \right\} - i \sin\left(\frac{2\pi\ell}{N}\right) \left\{ \underset{\sim}{G} - \underset{\sim}{G}^\dagger \right\} . \tag{14}$$

If we choose $\ell = \ell(N) = \pm\lceil N/2 \rceil$, then $\cos\left(\frac{2\pi\ell}{N}\right)$ is as close to -1 as possible. We will use the short-hand notation $\underset{\sim}{H}_\mathrm{B} \equiv \widehat{\underset{\sim}{H}}(\lceil N/2 \rceil)$ and equation (12) then yields a relation between the eigenstates of $\underset{\sim}{H}_\mathrm{B}$ and $\underset{\sim}{H}$: If any eigenstate $|\,\Psi_B\,\rangle$ of $\underset{\sim}{H}_\mathrm{B}$ has the shift quantum number k_B then the corresponding eigenstate of the original Hamiltonian has the shift quantum number $k = k_B - a\lceil N/2 \rceil$.

Consequently the k-rule 1 is equivalent to

k-rule 2 *For $N \neq 3$ the relative ground states of $\underset{\sim}{H}_B$ have the shift quantum numbers*

$$k = \begin{cases} 0 \mod N & : \ N \text{ even} \\ 0, a \mod N & : \ N \text{ odd} \end{cases} . \tag{15}$$

Their degeneracy is minimal.

For later use we also define a "Frobenius-Perron" Hamiltonian as

$$\underset{\sim}{H}_\mathrm{FP}(x) = \underset{\sim}{\Delta} + x \left\{ \underset{\sim}{G} + \underset{\sim}{G}^\dagger \right\} , \tag{16}$$

where x is an arbitrary real number. For negative x the operator (16) satisfies the conditions of the theorem of Frobenius and Perron[15] with respect to the product basis. We will utilize the following version of this theorem, adapted to the needs of physicists:

Let a symmetric matrix $\mathcal{A}$ have off-diagonal elements ≤ 0. Moreover, let $\mathcal{A}$ be *irreducible*, which means that every matrix element of $\mathcal{A}^n$ is non-zero for sufficiently high powers n of $\mathcal{A}$. Then $\mathcal{A}$ has a non-degenerate ground state with positive components.

Thus, in our case and for odd N the ground state of $\underset{\sim}{H}_\mathrm{FP}(x)$ will have the shift quantum number $k = 0$.

The Bloch transform for even N results in a pure Frobenius-Perron Hamiltonian, i. e. $\underset{\sim}{H}_\mathrm{B} = \underset{\sim}{H}_\mathrm{FP}(-1)$, whereas for odd N one obtains

$$\underset{\sim}{H}_\mathrm{B} = \underset{\sim}{H}_\mathrm{FP}(-\cos\left(\frac{\pi}{N}\right)) - i \sin\left(\frac{\pi}{N}\right) \left\{ \underset{\sim}{G} - \underset{\sim}{G}^\dagger \right\} . \tag{17}$$

III. CONSEQUENCES OF THE K-RULE

In the following we only consider the new case of odd N since the respective relations for even N are already known for a long time.[1–3]

Subspaces $\mathcal{H}(M)$ and $\mathcal{H}(M')$ are named "adjacent" if $M' = M - 1$ or, equivalently, $a' = a + 1$. The ordinary k-numbers for the respective relative ground states are $k = \pm a\lceil N/2 \rceil \mod N$ and $k' = \pm(a+1)\lceil N/2 \rceil \mod N$. As mentioned above these quantum numbers are different unless N divides $2a + 1$.

Relative ground states can be chosen to be eigenstates of $\underset{\sim}{\vec{S}}^2$. As we are going to show, the k-rule helps to understand that the total spin quantum number S of a relative ground state in $\mathcal{H}(M \geq 0)$ is $S = M$ not only for even N but also for odd N.

Let us consider $M' = Ns - (a+1) \geq 0$ and let $|\,\phi_k(a+1)\,\rangle$ be a ground state in $\mathcal{H}(M')$. If this state vanishes on applying the total ladder operator $\underset{\sim}{S}^+ = \sum_i \underset{\sim}{s}_i^+$, it is an eigenstate of $\underset{\sim}{\vec{S}}^2$ with $S = M' = Ns - (a+1)$.

The question is now whether $\underset{\sim}{S}^+\,|\,\phi_k(a+1)\,\rangle \neq 0$ is possible? If so, the resulting state would be an eigenstate of the shift operator $\underset{\sim}{T}$ with the same k-number, i. e. $k = \pm(a+1)\lceil N/2 \rceil$. But on the other hand the resulting state is also a ground state in $\mathcal{H}(M = Ns - a)$, because all the energy eigenvalues in $\mathcal{H}(M = Ns - a)$ are inherited by $\mathcal{H}(M' = Ns - (a+1))$. Then, the k-rule applies, but now for a instead of $(a+1)$, which produces a contradiction unless for those cases where N divides $(2a+1)$. In the latter cases one cannot exclude that the relative ground state energies $E_\mathrm{min}(M)$ and $E_\mathrm{min}(M')$ are the same.

We thus derive an S-rule from the k-rule for odd N:

- If N does not divide $(2a+1)$, then any relative ground state in $\mathcal{H}(M = Ns-(a+1))$ has the total spin quantum number $S = |M|$. In accordance the minimal energies fulfill $E_{\rm min}(M=S) < E_{\rm min}(M = S+1)$.
- For the absolute ground state with $a+1 = Ns$ or $a+1 = Ns-1/2$, N does never divide $(2a+1)$. The k-rule therefore yields, that the total spin of the absolute ground state is $S = 0$ for Ns integer and $S = 1/2$ for Ns half integer.

As an example we would like to discuss the case of $N = 5$ and $s = 1$, compare Table I. The magnon vacuum $a = 0$ has the total magnetic quantum number $M = Ns = 5$, $k = 0$, and $S = Ns = 5$. The adjacent subspace with $a = 1$ has $M = 4$ and $k = 2,3$, therefore, the ground state in this subspace must have $S = 4$. If the ground state had $S = 5$ it would already appear in the subspace "above". The next subspace belongs to $a = 2$, i. e. $M = 3$. It again has a different k, thus $S = 3$. While going to the next subspace $\mathcal{H}(M)$ the k-number does not change. Therefore, we cannot use our argument. We only know that the minimal energy in this subspace is smaller than or equal to that of the previous subspace. Going further down in M the k-values of adjacent subspaces are again different, thus $S = |M|$ and $E_{\rm min}(M = S) < E_{\rm min}(M = S+1)$.

IV. PROOFS FOR SPECIAL CASES

A. The case $a = 1$

The eigenvalues of the Hamiltonian in the subspace with $a = 1$ are well-known:

$$\begin{aligned} E_k &= 2Ns^2 - 4s + 4s\cos\frac{2\pi k}{N} \ , \\ & k = 0, 1, \dots, N-1 \ , \end{aligned} \tag{18}$$

where k is the corresponding shift quantum number. Obviously, the relative ground state is obtained for $k = \frac{N}{2}$ for even N and $k = \frac{N\pm 1}{2}$ for odd N.

B. The ground state of odd $s = 1/2$ rings

In this case the ground state belongs to $a = \frac{N-1}{2}$ and the k-rule (1) reads

$$k = \pm a^2 \mod N = \pm\left(\frac{N-1}{2}\right)^2 \mod N \ . \tag{19}$$

This now is an immediate consequence of the Bethe ansatz as we will show. Following the notation of Ref. 16, chapter 9.3, the energy eigenvalues in the subspace with $M = 1/2$ may be written as

$$E = 2\epsilon - N/2, \tag{20}$$

with

$$\epsilon = \sum_{i=0}^{a} (1-\cos f_i) \tag{21}$$

and

$$N f_i = 2\pi\lambda_i + \sum_j \varphi_{ij} \ , \tag{22}$$

where the λ_i are natural numbers between 0 and $N-1$ satisfying $|\lambda_i - \lambda_j| \geq 2$ for $i \neq j$ and the φ_{ij} are the entries of some antisymmetric phase matrix. Hence the two ground state configurations are $\vec{\lambda} = (1,3,5,\dots,N-2)$ and $\vec{\lambda}' = (2,4,6,\dots,N-1) = -\vec{\lambda} \mod N$. According to Ref. 16, p. 137, the shift quantum number of the ground state will be

$$k = \sum_j \lambda_j = \pm a^2 \mod N \ , \tag{23}$$

in accordance with (19).

C. The case $N = 3$

In this subsection we want to prove that the shift quantum numbers k of relative ground states satisfy the rule

$$k = \begin{cases} 1,2 & : \ a = 1 \\ 0 & : \ a = 3s, s \text{ integer} \\ 1,2 & : \ a = 3s-1/2, s \text{ half integer} \\ 0,1,2 & : \ \text{else} \end{cases} \ . \tag{24}$$

By completing squares the Hamiltonian can be written in the form

$$\underset{\sim}{H} = \underset{\sim}{\vec{S}}^2 - 3s(s+1) \tag{25}$$

and can be diagonalized in terms of Racah $6j$-symbols. The lowest eigenvalues in $\mathcal{H}(M)$ are those with $S = M = 3s-a$. In order to determine the shift quantum numbers of the corresponding eigenvectors we may employ the results in Ref. 17 on the dimension of the spaces $\mathcal{H}_N(M,S,k)$. Using equations (11) and (12) of Ref. 17 we obtain after some algebra

$$\dim(\mathcal{H}_3(M, S = M)) = \begin{cases} a+1 & : \ 0 \leq a \leq 2s \\ 6s-2a+1 & : \ 2s \leq a \leq \lfloor 3s \rfloor \end{cases} \ . \tag{26}$$

Now consider $\dim(\mathcal{H}_3(M,k))$. The product basis in $\mathcal{H}_3(M)$ may be grouped into $\nu(a)$ proper cycles of three different states $\{\,|\,\vec{m}\,\rangle, \underset{\sim}{T}\,|\,\vec{m}\,\rangle, \underset{\sim}{T}^2\,|\,\vec{m}\,\rangle\}$, and, if $a = 0 \mod 3$, one additional state $|\,\lambda,\lambda,\lambda\,\rangle$ having $k = 0$. Each 3-dimensional subspace spanned by a cycle contains a basis of eigenvectors of $\underset{\sim}{T}$ with each shift quantum number

$k=0,1,2$ occuring exactly once, hence

$$\dim\quad(\mathcal{H}_3(M,k)) = \qquad (27)$$
$$\begin{cases} \nu(a) & : \quad a\neq 0 \mod 3 \\ \nu(a) & : \quad k=1,2 \text{ and } a=0 \mod 3 \\ \nu(a)+1 & : \quad k=0 \text{ and } a=0 \mod 3. \end{cases} .$$

Note further that $\underset{\sim}{S}^- : \mathcal{H}(M) \longrightarrow \mathcal{H}(M-1)$ commutes with $\underset{\sim}{T}$, hence maps eigenvectors of $\underset{\sim}{T}$ onto eigenvectors with the same shift quantum number. This leads to

$$\dim(\mathcal{H}_3(M\ ,\ S=M,k)) = \qquad (28)$$
$$\begin{cases} \mu(a)+1 & : \quad k=0, a=0 \mod 3 \\ \mu(a)-1 & : \quad k=0, a=1 \mod 3 \\ \mu(a) & : \quad k=0, a=2 \mod 3 \\ \mu(a) & : \quad k=1,2 \end{cases} ,$$

with

$$\mu(a) \equiv \begin{cases} 0 & : \quad a=0 \\ \nu(a)-\nu(a-1) & : \quad a>0 \end{cases} . \qquad (29)$$

Comparison with (26) yields those values of a and s where $\dim(\mathcal{H}_3(M,S=M,k))$ vanishes for some k, i. e. where not all possible shift quantum numbers occur for the relative ground states. Due to (28) this happens if $\mu(a)=0$ or $\mu(a)=1$.

For $a=1$ only the values $k=1,2$ appear according to subsection IV A, hence $\mu(a)=1$. If s is integer and $a=3s$, (26) yields $\dim(\mathcal{H}_3(M=0,S=0))=1$, hence only $k=0$ appears for the ground state and $\mu(a)=0$. If s is half integer and $a=3s-1/2$, (26) yields $\dim(\mathcal{H}_3(M=1/2,S=1/2))=2$, hence only $k=1,2$ appear for the ground state and $\mu(a)=1$. For all other cases, $\mu(a)>1$ and all shift quantum numbers $k=0,1,2$ occur. This completes the proof of (24).

D. $a=2$ and odd N

In this subsection all states considered will be in the subspace $\mathcal{H}(M=Ns-2)$, N being odd. We will prove a weaker statement than k-rule 1, namely

k-rule 3 *If there are relative ground states of* $\underset{\sim}{H}$ *with* $k\neq 0$ *then there are exactly two such states with* $k=1$ *and* $k=-1$.

We think that the possibility $k=0$ can be excluded for $N>3$, but the proof of this apparently requires a more detailed analysis of the energy spectrum and will be published elsewhere. The situation in the case $a=2$ is greatly simplified due to the following fact

$$\underset{\sim}{T}\,|\,\psi\,\rangle = |\,\psi\,\rangle \quad \Rightarrow \quad \underset{\sim}{G}\,|\,\psi\,\rangle = \underset{\sim}{G}^\dagger\,|\,\psi\,\rangle\ . \qquad (30)$$

To prove this we define the unitary reflection operator $\underset{\sim}{R}$ by linear extension of

$$\underset{\sim}{R}\,|\,m_1,m_2,\ldots,m_N\,\rangle \equiv |\,m_N,m_{N-1},\ldots,m_1\,\rangle\ . \qquad (31)$$

Obviously,

$$\underset{\sim}{R}\underset{\sim}{G}\underset{\sim}{R} = \underset{\sim}{G}^\dagger\ . \qquad (32)$$

For $a=2$ any reflected product state can also be obtained by a suitable shift, i. e.

$$\underset{\sim}{R}\,|\,\vec{m}\,\rangle = \underset{\sim}{T}^{n(\vec{m})}\,|\,\vec{m}\,\rangle\ . \qquad (33)$$

Hence $\underset{\sim}{R}$ maps any cycle $\{\,|\,\vec{m}\,\rangle, \underset{\sim}{T}\,|\,\vec{m}\,\rangle,\ldots,\underset{\sim}{T}^{N-1}\,|\,\vec{m}\,\rangle\}$ onto itself and thus leaves states $|\,\psi\,\rangle$ with $\underset{\sim}{T}\,|\,\psi\,\rangle = |\,\psi\,\rangle$, i. e. with shift quantum number $k=0$, invariant. Now assume $\underset{\sim}{T}\,|\,\psi\,\rangle = |\,\psi\,\rangle$. We conclude $\underset{\sim}{G}^\dagger\,|\,\psi\,\rangle = \underset{\sim}{R}\underset{\sim}{G}\underset{\sim}{R}\,|\,\psi\,\rangle = \underset{\sim}{R}\underset{\sim}{G}\,|\,\psi\,\rangle = \underset{\sim}{G}\,|\,\psi\,\rangle$, since $\underset{\sim}{T}\underset{\sim}{G}\,|\,\psi\,\rangle = \underset{\sim}{G}\underset{\sim}{T}\,|\,\psi\,\rangle = \underset{\sim}{G}\,|\,\psi\,\rangle$. This concludes the proof of (30).

In the following $E_{\text{FP}}(x)$ denotes the lowest eigenvalue of the Frobenius-Perron Hamiltonian $\underset{\sim}{H}_{\text{FP}}(x)$ as defined by Eq. 16. Since $[\underset{\sim}{H}_{\text{FP}}(x),\underset{\sim}{T}]=0$ there exists a complete system of simultaneous eigenvectors of $\underset{\sim}{H}_{\text{FP}}(x)$ and $\underset{\sim}{T}$. Especially, for $x<0$ the eigenvector corresponding to $E_{\text{FP}}(x)$ will have positive components in the product basis (4) and hence the shift quantum number $k=0$.

By using arguments based on the Ritz variational principle one shows easily

$$x<y<0 \quad \Rightarrow \quad E_{\text{FP}}(x) < E_{\text{FP}}(y)\ , \qquad (34)$$

and

$$x\neq 0 \quad \Rightarrow \quad E_{\text{FP}}(-|x|) < E_{\text{FP}}(|x|)\ . \qquad (35)$$

Equivalent to k-rule 3 is the corresponding statement on $\underset{\sim}{H}_{\text{B}}$: If there are relative ground states of $\underset{\sim}{H}_{\text{B}}$ with $k_{\text{B}}\neq 1$, then there are exactly two such states with $k_{\text{B}}=0$ and $k_{\text{B}}=2$.

Note that in our case $k_{\text{B}} = k + 2\frac{N+1}{2} = k+1 \mod N$. Due to (17) and (30) $\underset{\sim}{H}_{\text{B}}$ equals $\underset{\sim}{H}_{\text{FP}}(-\cos\frac{\pi}{N})$, if restricted to the sector $k=0$. The ground state in this sector is non-degenerate according to the theorem of Frobenius-Perron and will be denoted by $|\,\Phi\,\rangle$. It remains to show that

(A) $|\,\Phi\,\rangle$ is also a ground state of $\underset{\sim}{H}_{\text{B}}$ in the whole subspace $\{k_{\text{B}}=1\}^\perp$ which is orthogonal to the $k_{\text{B}}=1$ sector, and

(B) any other relative ground state of $\underset{\sim}{H}_{\text{B}}$ has $k_{\text{B}}=1$ or $k_{\text{B}}=2$.

The relative ground state of $\underset{\sim}{H}_{\text{B}}$ with $k_{\text{B}}=2$ will then be non-degenerate too. This is easily proven by retranslating into the $\underset{\sim}{H}$-picture and employing the $+k \leftrightarrow -k$ symmetry.

In order to prove (A) we consider an arbitrary eigenvalue E of $\underset{\sim}{H}_{\text{B}}$ in $\mathcal{H}(M=Ns-2)$ which does not comply with the shift quantum number $k_{\text{B}}=1$. We have to show that

$$E \geq E_{\text{FP}}(-\cos\frac{\pi}{N})\ . \qquad (36)$$

E is also an eigenvalue of $\underset{\sim}{H}$ corresponding to an eigenvector $|\,\psi\,\rangle$ with shift quantum number $k \neq 0$. Since N is odd, there exists an integer $\ell \neq 0$, unique modulo N, such that $2\ell = N - k \mod N$. According to (12), $|\,\phi\,\rangle \equiv \underset{\sim}{U}^{\ell}\,|\,\psi\,\rangle$ satisfies

$$\underset{\sim}{T}\,|\,\phi\,\rangle = |\,\phi\,\rangle, \tag{37}$$

and, using (14) together with (30),

$$\underset{\sim}{U}^{\ell}\underset{\sim}{H}\underset{\sim}{U}^{\dagger\ell}\,|\,\phi\,\rangle = E\,|\,\phi\,\rangle = \underset{\sim}{H}_{\mathrm{FP}}(\cos\alpha\ell)\,|\,\phi\,\rangle\ , \tag{38}$$

where $\alpha \equiv 2\pi/N$. Hence

$$E \geq E_{\mathrm{FP}}(\cos\alpha\ell)\ , \tag{39}$$

by the definition of $E_{\mathrm{FP}}(x)$. If $\cos\alpha\ell > 0$, (34) and (35) yield

$$\begin{aligned} E_{\mathrm{FP}}(\cos\alpha\ell) \ &\geq\ E_{\mathrm{FP}}(-\cos\alpha\ell) \\ &= E_{\mathrm{FP}}(\cos(\pi - \alpha\ell)) \geq E_{\mathrm{FP}}(-\cos\frac{\pi}{N})\ , \end{aligned} \tag{40}$$

since $\ell \neq 0$. For $\cos\alpha\ell < 0$ the analogous inequality follows directly from (34). Hence

$$E \geq E_{\mathrm{FP}}(-\cos\frac{\pi}{N})\ , \tag{41}$$

and the proof of (A) is complete.

Turning to the proof of (B) we note that, because of the strict inequalities (34) and (35), $E = E_{\mathrm{FP}}\,(\cos\alpha\ell) = E_{\mathrm{FP}}\left(-\cos\frac{\pi}{N}\right)$ is only possible if

$$\cos\frac{2\pi\ell}{N} \ =\ \cos\alpha\ell = -\cos\frac{\pi}{N}\ . \tag{42}$$

Using $2\ell = N - k \bmod N$, after some elementary calculations this can be shown to be equivalent to

$$k \ =\ \pm 1 \bmod N\ , \tag{43}$$

i. e.

$$k_{\mathrm{B}} \ =\ 0, 2 \bmod N\ , \tag{44}$$

which completes the proof of (B) and k-rule 3.

E. Haldane systems

One idea to prove part of the k-rule 2 for odd N would be to show that one of the relative ground states has an overlap with another eigenstate of the shift operator whose shift quantum number is known to be zero. A good candidate would be the relative ground state of $\underset{\sim}{H}_{\mathrm{FP}}(-\cos\pi/N)$ (16) in $\mathcal{H}(M)$ which has $k = 0$. If this state has overlap with a relative ground state of $\underset{\sim}{H}_{\mathrm{B}}$ (17) the latter also possesses $k = 0$.

Let $\underset{\sim}{V} = \underset{\sim}{U}^{(N+1)/2}$, $|\,\Psi_0\,\rangle$ and $|\,\hat{\Psi}_0\,\rangle = \underset{\sim}{V}\,|\,\Psi_0\,\rangle$ be one of the relative ground states of $\underset{\sim}{H}$ (2) and $\underset{\sim}{H}_{\mathrm{B}}$ (14), respectively. $|\,\Psi_{\mathrm{FP}}\,\rangle$ denotes the relative ground state of $\underset{\sim}{H}_{\mathrm{FP}}$. Then part of the k-rule is implied by the following

k-rule 4 *$|\,\Psi_{FP}\,\rangle$ has a non-vanishing $\underset{\sim}{H}_B$-ground-state component, i. e. $\langle\,\Psi_{FP}\,|\,\hat{\Psi}_0\,\rangle \neq 0$.*

The validity of this k-rule would immediately follow from the sufficient (but not necessary) inequality

$$E_{\mathrm{FP}} - E_0 \ <\ E_1 - E_0\ , \tag{45}$$

where E_1 is the energy of the first excited state above the relative ground state in $\mathcal{H}(M)$ and

$$E_{\mathrm{FP}} = \langle\,\Psi_{\mathrm{FP}}\,|\,\underset{\sim}{H}_{\mathrm{B}}\,|\,\Psi_{\mathrm{FP}}\,\rangle = \langle\,\Psi_{\mathrm{FP}}\,|\,\underset{\sim}{H}_{\mathrm{FP}}\,|\,\Psi_{\mathrm{FP}}\,\rangle\ . \tag{46}$$

As a substitute for the lacking proof of k-rule 4 we submit the inequality (45) to some numerical tests, see section V.

Looking at the large N behavior it is nevertheless possible to devise an asymptotic proof for systems which possess a finite energy gap in the thermodynamic limit $N \to \infty$. These systems are called “Haldane systems”. According to Haldane's conjecture[18,19] spin rings with an integer spin quantum number s possess such gaps.

To start with the proof, let us look for an upper bound to $E_{\mathrm{FP}} - E_0$. Take $|\,\Psi_0\,\rangle$ to be a ground state of $\underset{\sim}{H}$ with real coefficients with respect to the product basis $\{\,|\,\vec{m}\,\rangle\}$. Evidently,

$$\begin{aligned} E_{\mathrm{FP}} \ &\leq\ \langle\,\Psi_0\,|\,\underset{\sim}{V}^{\dagger}\underset{\sim}{H}_{\mathrm{FP}}\underset{\sim}{V}\,|\,\Psi_0\,\rangle \\ &\leq\ E_0 + i\sin\left(\frac{\pi}{N}\right) \\ &\qquad \times\langle\,\Psi_0\,|\,\underset{\sim}{V}^{\dagger}\left\{\underset{\sim}{G} - \underset{\sim}{G}\right\}\underset{\sim}{V}^{\dagger}\,|\,\Psi_0\,\rangle\ . \end{aligned} \tag{47}$$

Further, in view of (13)

$$\underset{\sim}{V}^{\dagger}\left\{\underset{\sim}{G} - \underset{\sim}{G}^{\dagger}\right\}\underset{\sim}{V} \ =\ -\left\{\mathrm{e}^{i\frac{\pi}{N}}\underset{\sim}{G} - \mathrm{e}^{-i\frac{\pi}{N}}\underset{\sim}{G}^{\dagger}\right\}\ , \tag{48}$$

and, because $\langle\,\vec{m}\,|\,\Psi_0\,\rangle$ being real, $\langle\,\Psi_0\,|\,\underset{\sim}{G} - \underset{\sim}{G}^{\dagger}\,|\,\Psi_0\,\rangle = 0$. Therefore,

$$E_{\mathrm{FP}} - E_0 \ \leq\ \sin^2\left(\frac{\pi}{N}\right)\langle\,\Psi_0\,|\,\underset{\sim}{G} + \underset{\sim}{G}^{\dagger}\,|\,\Psi_0\,\rangle\ . \tag{49}$$

A rough upper estimate for the operator norm of $\{\underset{\sim}{G} + \underset{\sim}{G}^{\dagger}\}$ in $\mathcal{H}(M = Ns - a)$ can be deduced from the well-known Geršgorin bounds for matrix eigenvalues (c. f.[15], 7.2):

$$||\underset{\sim}{G} + \underset{\sim}{G}^{\dagger}|| \leq 2\,f(s)\,\min(a, N, 2Ns - a)\ , \tag{50}$$

where

$$f(s) \ =\ \begin{cases} (s + \frac{1}{2})^2 & s \text{ half integer} \\ (s + \frac{1}{2})^2 - \frac{1}{4} & s \text{ integer} \end{cases}\ . \tag{51}$$

We therefore conclude

$$E_{\mathrm{FP}} - E_0 \ \leq\ 2\,N\,\sin^2\left(\frac{\pi}{N}\right)f(s)\ . \tag{52}$$

Thus, with increasing N, $(E_{\mathrm{FP}} - E_0)$ approaches zero at least like $1/N$ and therefore, above some N_0, $(E_{\mathrm{FP}} - E_0)$ must be smaller than the Haldane gap $(E_1 - E_0)$.

One would of course like to accomplish a similar proof for half integer spin systems, but in this case $(E_1 - E_0)$ drops like $1/N$ itself as given by the Wess-Zumino-Witten model, see e.g. Ref. 13. Thus for such systems a careful analysis of the coefficient in front of the $1/N$ might be very valuable. As shown in the next section, numerical investigations indicate that $(E_{\mathrm{FP}} - E_0)$ approaches zero faster than $(E_1 - E_0)$.

V. NUMERICAL STUDIES

s	$N=3$	5	7	9	11	
$\frac{1}{2}$	-1.5	-3.736	-5.710	-7.595	-9.438	E_0
	-1.5	-3.736	-5.706	-7.589	-9.431	E_{FP}
	1.5	-1.5	-3.612	-5.872	-7.984	E_1
1	-6.0	-13.062	-19.144	-24.960	-30.67	E_0
	-5.162	-12.180	-18.338	-24.235	-30.02	E_{FP}
	-4.0	-11.133	-17.431	-23.420	-29.26	E_1
$\frac{3}{2}$	-10.5	-24.865	-37.370	-49.296	$-60.98^{\dagger}$	E_0
	-9.788	-24.095	-36.663	-48.658	$-60.40^{\dagger}$	E_{FP}
	-7.5	-22.237	-35.199	-47.458	$-59.38^{\dagger}$	E_1
2	-18.0	-42.278	-63.315	$-83.364^{\dagger}$	$-103.0^{\dagger\dagger}$	E_0
	-16.506	-40.615	-61.789	$-81.989^{\dagger}$	$-101.8^{\dagger\dagger}$	E_{FP}
	-16.0	-40.356	-61.663	$-81.934^{\dagger}$	$-101.7^{\dagger\dagger}$	E_1
$\frac{5}{2}$	-25.5	-62.168	-94.160	$-124.63^{\dagger}$	$-154.4^{\dagger\dagger}$	E_0
	-24.188	-60.699	-92.814	$-123.42^{\dagger}$	$-153.3^{\dagger\dagger}$	E_{FP}
	-22.5	-59.538	-92.006	$-122.83^{\dagger}$	$-152.9^{\dagger\dagger}$	E_1
3	-36.0	-87.666	$-132.68^{\dagger}$	$-175.55^{\dagger}$	$-217.5^{\dagger\dagger}$	E_0
	-33.936	-85.325	$-130.55^{\dagger}$	$-173.66^{\dagger}$	$-215.8^{\dagger\dagger}$	E_{FP}
	-34.0	-85.747	$-131.06^{\dagger}$	$-174.18^{\dagger}$	$-216.3^{\dagger\dagger}$	E_1

TABLE II: Lowest energy eigenvalues of the Heisenberg Hamiltonian (E_0,E_1) as well as of the respective Frobenius-Perron Hamiltonian (E_{FP}) for various odd N and s; † – projection method,[20] †† – Lánczos method. Note that we find $E_0 \leq E_{\mathrm{FP}} < E_1$ for all N if $s \leq 5/2$. Except for $N = 5, s = 1/2$ the first excited state has a higher total spin than the ground state, i.e. $S_1 = S_0 + 1$.

The question (45) whether $(E_{\mathrm{FP}} - E_0) < (E_1 - E_0)$ holds in $\mathcal{H}(M)$ with minimal $|M|$ was investigated numerically. For some of the investigated rings the respective energies are given in Table II.

Figure 1 shows the ratio $(E_{\mathrm{FP}}-E_0)/(E_1-E_0)$ for rings with $s = 1/2, \ldots, 3$ and various N. This ratio is smaller than one for $s = 1/2, 1, 3/2, 5/2$ for all investigated N. Only for $s = 2, 3$ the ratio reaches values above one. Nevertheless, as discussed in the previous section, in the cases of integer s this ratio must approach zero like $1/N$ if $(E_1 - E_0)$ tends to a nonzero Haldane gap. But also in the cases of half integer spin one is led to anticipate that

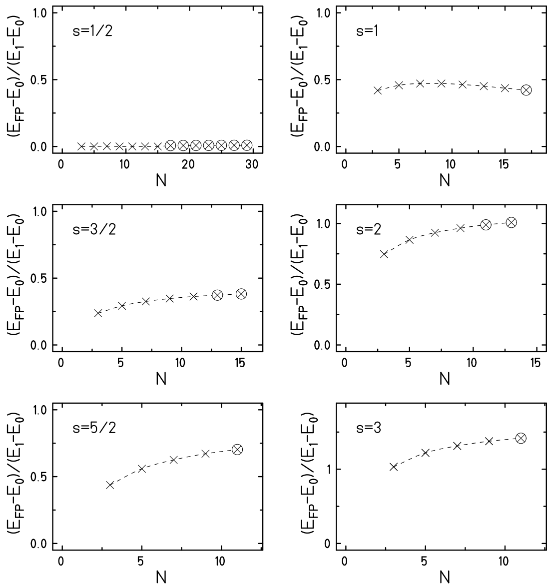

FIG. 1: Dependence of $(E_{\mathrm{FP}}-E_0)/(E_1-E_0)$ on N for various s. Crosses denote values obtained by exact diagonalization or projection method, circled crosses denote values obtained by a Lánczos method. For $s = 1/2$, where $[\underset{\sim}{G}, \underset{\sim}{G}^{\dagger}] = 0$, the ratio $(E_{\mathrm{FP}} - E_0)/(E_1 - E_0)$ is extremely small, i. e. $\approx 10^{-2}$.

the ratio $(E_{\mathrm{FP}}-E_0)/(E_1-E_0)$ remains smaller than one and that the curves rising with N for small N might even bend down later and approach zero for large N. DMRG calculations could help to clarify this question.

VI. GENERALIZATION TO OTHER SPIN MODELS

It is a legitimate question whether the k-rule holds for Heisenberg spin rings only or whether it is valid for a broader class of spin Hamiltonians. In order to clarify this question we investigate the following XXZ-Hamiltonian

$$\underset{\sim}{H}(\delta) \;=\; \delta \cdot \underset{\sim}{\Delta} + \underset{\sim}{G} + \underset{\sim}{G}^{\dagger} \;, \qquad (53)$$

for various values of δ. The case $\delta = 1$ corresponds to the original Heisenberg Hamiltonian (6), $\delta \to \infty$ results in the antiferromagnetic Ising model, $\delta \to -\infty$ in the ferromagnetic Ising model, and $\delta = 0$ describes the XY-model.

We have numerically investigated the cases of $\delta = -1000, -1, 0, 0.5, 1000$ for $s = 1/2, \ldots, 5/2$ and $N = 5, \ldots, 8$. For $|\delta| \leq 1$ no violation of the k-rule was found, whereas the k-rule is violated for $\delta = \pm 1000$.

In the limiting case of the Ising model the k-rule 1 is in general violated. Any product state $|\,\vec{m}\,\rangle$ will be an eigenstate of the Ising Hamiltonian and the shifted states $\underset{\sim}{T}^{\nu}\,|\,\vec{m}\,\rangle$ belong to the same eigenvalue $E_{\vec{m}}$. The set of the corresponding shift quantum numbers then depends on the degree of symmetry of $|\vec{m}\rangle$: Let n denote the smallest positive integer such that $\underset{\sim}{T}^n |\vec{m}\rangle = |\vec{m}\rangle$. Clearly, n divides N. Then the corresponding shift quantum numbers will be of the form $k = \frac{N}{n}\ell \mod N,\ \ell = 0, 1, 2, \ldots$. In most cases, $n = N$ and hence all possible shift quantum numbers will occur, which violates 1. On the other hand consider the total ground state $|\uparrow, \downarrow, \uparrow, \downarrow, \ldots\rangle$ of an even $s = 1/2$ antiferromagnetic Ising spin ring. Here we have $n = 2$ and only the shift quantum numbers $k = 0, \frac{N}{2}$ occur, also contrary to 1. Figure 2 summarizes our findings as a graphics.

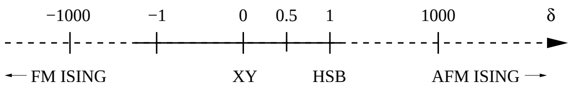

FIG. 2: Solid line: Estimated validity of the k-rule for various parameters δ of the Hamiltonian (53). The numbers denote the cases which have been examined numerically. The k-rule is violated for $\delta = \pm 1000$, no violation was found for $|\delta| \leq 1$.

It is not clear at which δ exactly the k-rule breaks down. This quantum phase transition might very well depend on N and s. It is then an open question whether another k-rule takes over.

Finally we would like to mention that the exactly solvable $s = 1/2$ XY-model[2,21] satisfies the k-rule (1). This model is essentially equivalent to a system of a non-interacting Fermions. More precisely, for odd a its energy eigenvalues are of the form

$$E^{(\text{odd})}_{\vec{k}} = 2\sum_{\nu=1}^{a} \cos\left(\frac{2\pi}{N} k_\nu\right) \ , \ k_\nu \text{ integer} \ , \qquad (54)$$

with corresponding shift quantum numbers

$$k = \sum_{\nu=1}^{a} k_\nu \mod N \ . \qquad (55)$$

Relative ground state configurations $\vec{k}$ for $a = 1, 3, 5, \ldots$ and odd N are, for example,

$$\vec{k} = \left(\frac{N+1}{2}\right), \left(\frac{N\pm 1}{2}, \frac{N+3}{2}\right), \left(\frac{N\pm 1}{2}, \frac{N\pm 3}{2}, \frac{N+5}{2}\right) \ldots \qquad (56)$$

This leads to the shift quantum numbers

$$k = \frac{N+1}{2}, \frac{N+3}{2}, \frac{N+5}{2}, \ldots \qquad (57)$$

in accordance with (1). Similarly, the values

$$k = \frac{N-1}{2}, \frac{N-3}{2}, \frac{N-5}{2}, \ldots \qquad (58)$$

are realized. In the case of even a we have

$$E^{(\text{even})}_{\vec{k}} = 2\sum_{\nu=1}^{a} \cos\left(\frac{2\pi}{N}\frac{2k_\nu + 1}{2}\right) \ , \ k_\nu \text{ integer} \ , \qquad (59)$$

with corresponding shift quantum numbers

$$k = \sum_{\nu=1}^{a} \left(k_\nu + \frac{1}{2}\right) \mod N \ , \qquad (60)$$

and the k-rule 1 follows analogously.

Acknowledgments

We thank Shannon Starr for motivating discussions and Ian Affleck for pointing out some useful literature.

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