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# Energy Gaps and Elementary Excitations for Certain VBS-Quantum Antiferromagnets

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It is shown for a class of antiferromagnetic Hamiltonians how one can get lower bounds for the energy gap above the ground state by diagonalizing a finite system. This method is applied to certain spin chains (including a spin-1 chain). Trial wave functons are proposed for the elementary excitations and are tested in the case of the spin-1 chain.

**KEY WORDS:** Quantum antiferromagnets; valence-bond ground states; energy gap; elementary excitations.

## 1. INTRODUCTION

For the ground state properties of the isotropic Heisenberg antiferromagnetic spin chain it seems to be crucial whether the spin per site is half-integral or integral. Whereas for half-integral spin a gapless ground state is expected, Haldane[1] argued that in the integral case a gap immediately above the ground state occurs.

The first rigorous result was obtained in ref. 2 for spin 1 if one replaces the usual Heisenberg interacton $S_i \cdot S_{i+1}$ by the projection $P_2(S_i, S_{i+1})$ on the two spin states with total spin 2. If one makes this replacement, one can calculate the exact ground state (called VBS state) and the ground state energy (namely, 0). The VBS state can be constructed for every lattice with coordination number $z$ if the spin per site is $S = z/2$ and the interaction is $P_{ij} = P_{2S}(S_i, S_j)$, the projection on the highest possible total spin of two neighboring spins.

Kennedy *et al.*[2,8] have shown the existence of the energy gap for the spin-1 chain and the exponential decay of the spin correlation function for

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the spin-1 chain, the hexagonal lattice (spin 3/2), and the square lattice (spin 2). Therefore one strongly believes that there is also an energy gap for the latter two lattices.

One can also consider systems with $S > z/2$. Again one knows all the ground states, but now the degeneracy of the ground state is infinite for the infinite system. In this paper I will show that there is an energy gap for the spin chains with spin $S = 1$, 3/2, 2, or 5/2 per site. More precisely, let

$$H_{S,N} = \sum_{i=1}^{N} P_{2S}(S_i, S_{i+1}) \tag{1.1}$$

where $S_{N+1} = S_1$, be the Hamiltonian for $N$ sites and periodic boundary conditions, and let $\varepsilon_{S,N}$ be the smallest eigenvalue larger than zero. We shall derive lower bounds for $\varepsilon_{S,N}$ independent of $N$. Affleck and Lieb[7] have shown for a wide class of Hamiltonians that for a chain with half-integral spin either there is no energy gap or the ground state is degenerate. Therefore our model (for $S = 3/2$ or 5/2) is an example where the second possibility is realized.

It is also interesting to get a good picture of the elementary excitations. In Section 3 I propose trial wave functions for them; the energy gap obtained by this approximation fits well with numerical results in the case of the spin-1 chain.

Let us now write down the form of the VBS states. For that it is convenient to use the following representation of the spin-$S$ states[10,3,4]: Consider the monomials in two variables

$$u^{2S-m} v^m, \qquad m = 0, 1, \ldots, 2S, \qquad u, v \in \mathbf{C} \tag{1.2}$$

It is easy to see that they span a space that is invariant and irreducible under $SU(2)$. The corresponding spin equals $S$. If we restrict the generators of $SU(2)$ to this space, then they can be written as

$$S^z = \frac{1}{2}\left(u\frac{\partial}{\partial u} - v\frac{\partial}{\partial v}\right), \qquad S^+ = u\frac{\partial}{\partial v}, \qquad S^- = v\frac{\partial}{\partial u} \tag{1.3}$$

The integration measure that has to be used is the $SO(4)$-invariant measure of $S^3 = \{(u, v) \in \mathbf{C}^2 \mid |u|^2 + |v|^2 = 1\}$, which is also $SU(2)$ invariant. However, for functions which are invariant under the $U(1)$ transform $(u, v) \mapsto (e^{i\alpha}u, e^{i\alpha}v)$, $\alpha \in \mathbf{R}$, we can carry out the integration over $S^2$ by using the solid angle representation

$$u = \cos\frac{\theta}{2} e^{i(\phi/2)}, \qquad v = \sin\frac{\theta}{2} e^{-i(\phi/2)} \tag{1.4}$$

The norms of the states in (1.2) can be calculated by the formula

$$\int_{S^2} |u|^{2k} |v|^{2l} \, d\Omega = \frac{k!\, l!}{(l+k)!\, (l+k+1)} \tag{1.5}$$

where $d\Omega$ is the $SO(3)$-invariant measure on $S^2$ normed by

$$\int_{S^2} d\Omega = 1 \tag{1.6}$$

namely $d\Omega = (1/4\pi) \sin\theta \, d\theta \, d\phi$. The space of $N$ spin-$S$ wave functions is now given by the polynomials $p(u_1, v_1, \ldots, u_N, v_N)$, which are homogeneous in every spin coordinate $(u_i, v_i)$ of degree $2S$. The coherent states of two spin-$S$ particles with total spin $\mathscr{S}$ are given by

$$(u_1 v_2 - v_1 u_2)^{2S-\mathscr{S}} \prod_{i=1}^{2} (\alpha^* u_i + \beta^* v_i)^{\mathscr{S}}, \qquad (\alpha, \beta) \in S^3 \tag{1.7}$$

and we get a basis of these states by expanding this expression in $\alpha$ and $\beta$ and taking the coefficients of $\alpha^{*\,2S-m} \beta^{*\,m}$.

Using (1.7) for $\mathscr{S} = 2S$, we see that

$$\begin{aligned} &P_{2S}(S_1, S_2) u_1^{m_1} v_1^{2S-m_1} u_2^{m_2} v_2^{2S-m_2} \\ &\quad = [1/\binom{4S}{m_1+m_2}] \sum_m \binom{2S}{m} \\ &\qquad \times \binom{2S}{m_1+m_2-m} u_1^m v_1^{2S-m} u_2^{m_1+m_2-m} v_2^{2S-(m_1+m_2-m)} \end{aligned} \tag{1.8}$$

where $m$ runs from $\max(0, m_1+m_2-2S)$ to $\min(2S, m_1+m_2)$.

Let us now consider a finite lattice $L$ with coordination number $z$ at each site, spin $S = z/2$ per site, and the Hamiltonian

$$H = \sum_{\langle i,j \rangle \in L} P_{2S}(S_i, S_j) \tag{1.9}$$

Now we claim that

$$\psi_0 = \prod_{\langle i,j \rangle \in L} (u_i v_j - v_i u_j) \tag{1.10}$$

is the unique ground state with eigenvalue zero.

From (1.7) we see that $H\psi_0 = 0$. Furthermore, $H \geqslant 0$, and from $H\psi = 0$ it follows again by (1.7) and by the unique factorization theorem[8]

that $\psi$ must be divisible by $\psi_0$. But since the degree per spin coordinate must be $z$, one must have $\psi = \text{const} \cdot \psi_0$. For the uniqueness of the ground state in the infinite lattice see refs. 2 and 8.

## 2. REDUCTION OF THE ENERGY GAP CALCULATION TO FINITE-SIZE CALCULATION

In this section I propose a method of getting lower bounds of energy gaps of infinite systems by diagonalizing finite systems. The method works if the energy gap of the finite system is larger than a certain value, which depends on the finite lattice. This value goes to zero if the size of the finite system goes to infinity.

Define the energy gap of the infinite system by considering a lattice with periodic boundary conditions and letting the size of the lattice go to infinity. The finite system I will diagonalize, however, will have free boundary conditions. I first illustrate the idea by considering the one-dimensional case.

Let the Hamiltonian $H$ be given by

$$H = \sum_{i=1}^{N} P_{i,i+1} \tag{2.1}$$

where $P_{i,i+1} = P(S_i, S_{i+1})$ acts on the two spins $S_i$ and $S_{i+1}$, $P$ is a projection operator and $S_{N+1} = S_1$ (periodic boundary conditions). If we know that zero is the ground state energy, then the energy gap is at least $\varepsilon$ if and only if

$$H^2 \geqslant \varepsilon H \tag{2.2}$$

My purpose is now to show such an inequality. If one squares $H$, one gets three types of terms, namely

$$P_{i,i+1}^2 = P_{i,i+1}, \quad P_{i+1,i+2} + P_{i+1,i+2} P_{i,i+1}, \quad 2P_{i,i+1} P_{j,j+1} \qquad (j \geqslant i+2)$$

The terms of the first and the third type are positive. However, this is not true for the terms of the second type.

Let us now assume that we already know that the Hamiltonian corresponding to a system of $n+1$ sites,

$$h_{n,i} = \sum_{j=i}^{i+n-1} P_{j,j+1} \tag{2.3}$$

where $P_{j,j+1} = P_{j+N,j+N+1}$, has the energy gap $\varepsilon_n$. Then

$$h_{n,i}^2 \geqslant \varepsilon_n h_{n,i} \tag{2.4}$$

holds. We will now try to get an inequality of the form

$$H^2 \geqslant \alpha \sum_{i=1}^{N} h_{n,i}^2 - \beta H \tag{2.5}$$

by adjusting $\alpha$ and $\beta$ such that we get equality for the terms of types 1 and 2.

Each term of type 2 appears $n-1$ times in $\sum_{i=n}^{N} h_{n,i}^2$, and therefore we must choose $\alpha = 1/(n-1)$. Since each term of type 1 appears $n$ times in $\sum_{i=n}^{N} h_{n,i}^2$, we must choose $\beta = 1/(n-1)$. Now every term of type 3 appears more often in the lhs of (2.5) than in the rhs, and therefore we get the inequality

$$H^2 \geqslant \frac{1}{n-1} \sum_{i=1}^{N} h_{n,i}^2 - \frac{1}{n-1} H \tag{2.6}$$

Using (2.4), we get

$$\begin{aligned} H^2 &\geqslant \frac{\varepsilon_n}{n-1} \sum_{i=n}^{N} h_{n,i}^2 - \frac{1}{n-1} H \\ &= \frac{n}{n-1} \varepsilon_n H - \frac{1}{n-1} H = \frac{n}{n-1} \left( \varepsilon_n - \frac{1}{n} \right) H \end{aligned} \tag{2.7}$$

Thus, *H has an energy gap (independent of N), if* $\varepsilon_n > 1/n$. Using the numerical results in Tables I and III, we have therefore proven the following.

**Theorem 2.1.** For spins $S = 1$, 3/2, 2, 5/2 the Hamiltonian $H_{S,N}$ has an energy gap in the limit $N \to \infty$, and the following lower bounds for the energy gaps $\varepsilon_{S,N}$ are valid:

$$\begin{aligned} \varepsilon_{1,N} &\geqslant 0.248064, & \varepsilon_{3/2,N} &\geqslant 0.141017 \\ \varepsilon_{2,N} &\geqslant 0.128138, & \varepsilon_{5/2,N} &\geqslant 0.121214 \end{aligned} \tag{2.8}$$

These estimates are not very good. The estimate for $S = 1$ is better than the others because we used the result for six sites for $S = 1$, but only for four sites in the other cases.

The generalization to lattices in more dimensions is straightforward. Let us, for instance, examine the hexagonal lattice. Define

$$H = \sum_{\langle i,j \rangle \in L} P_{ij} \tag{2.9}$$

where $L$ is a hexagonal lattice with torus boundary conditions. For every sublattice $Q$ let

$$h_Q = \sum_{\langle i,j\rangle \in Q} P_{ij} \tag{2.10}$$

As in the one-dimensional case, we obtain an inequality

$$H^2 \geqslant \alpha \sum_{\tau} h_{\tau(Q)}^2 - \beta H \tag{2.11}$$

with suitable chosen $\alpha$ and $\beta$ by considering the type 1 and type 2 terms. Here $\tau$ runs over all translations (and all possible rotations, if $Q$ is not rotatonally invariant). The three types of terms are now given by $P_{ij}$, $P_{ij}P_{jk} + P_{jk}P_{ij}$ $(i \neq k)$, $2P_{ij}P_{kl}$ ($\langle i,j\rangle$ and $\langle k,l\rangle$ disjoint). If $Q$ consists of three sites (one site joint with two others), we must choose $\alpha = 1$, $\beta = 3$ and we therefore get

$$H^2 \geqslant 4\varepsilon H - 3H = 4(\varepsilon - 3/4)H \tag{2.12}$$

where $\varepsilon$ is the energy gap of $h_Q$. This means that we need an energy gap $> 3/4$ for this system. The true energy gap, however is $1/2$.

The next simpler case consists of four sites (one site joined to three others). In this case we have to choose $\alpha = 1$, $\beta = 1$, and the energy gap we need is $> 1/2$. The true value, however, is $\approx 0.18$.

As the last example, consider sublattices $Q_n$, where $Q_1$ is a hexagon and $Q_n$ consists of $Q_{n-1}$ and all hexagons which touch $Q_{n-1}$.

The centers of the hexagons of $Q_n - Q_{n-1}$ form a hexagon with $n$ points per side. The number of these hexagons is $6(n-1)$; the number of boundary links is therefore $12n - 6$. The number of sites of $Q_n$ is $6n^2$. It is now easy to calculate that $\sum_\tau h_{\tau(Q_n)}^2$ (summation over all translations) contains every type 1 term $3n^2 - n$ times, every type 2 term $3n^2 - 2n$ times, and every type 3 term less than $3n^2 - 2n$ times. If $\varepsilon_n$ is the gap of $H_{Q_n}$, we get therefore

$$\begin{aligned} H^2 &\geqslant \frac{1}{3n^2-2n} \sum_{\tau} h_{\tau(Q_n)}^2 - \frac{n}{3n^2-2n} H \\ &\geqslant \left( \varepsilon_n \frac{3n^2-n}{3n^2-2n} - \frac{n}{3n^2-2n} \right) H = \frac{3n-2}{3n-1} \left( \varepsilon_n - \frac{1}{3n-1} \right) H \end{aligned} \tag{2.13}$$

The smallest $n$ such that $\varepsilon_n > 0.18$ is $n = 3$. But $Q_3$ has 54 sites, and that is much more than we can calculate on the computer.

In principle our method works if there exists an energy gap in the case of *free boundary conditions*. It could be, however, that there are gapless

excitations along the boundary. But the one-dimensional results seem to indicate that this is not the case. Furthermore, the exponential decay of spin correlation functions is true for all boundary conditions.[6]

## 3. ELEMENTARY EXCITATIONS

In this section we try to find good trial wave functions for the elementary excitations. Consider the same Hamiltonian as in Section 1 with periodic boundary condition and $S = z/2$. Then the ground state is unique, its total spin is zero, and is given by

$$\psi_0 = \prod_{\langle i,j\rangle \in L} (u_i v_j - v_i u_j) \tag{3.1}$$

Now we create a "crackion" at the link $\langle i, j\rangle$ by replacing the factor $(u_i v_j - v_i u_j)$ by $(\alpha^* u_i + \beta^* v_i)(\alpha^* u_j + \beta^* v_j)$:

$$\psi_{ij} := \frac{(\alpha^* u_i + \beta^* v_i)(\alpha^* u_j + \beta^* v_j)}{(u_i v_j - v_i u_j)} \psi_0 \qquad [(\alpha, \beta) \in S^3] \tag{3.2}$$

Here $(\alpha, \beta)$ is arbitrary but fixed. The crackion has spin 1 and therefore $\psi_{ij}$ is othogonal to the ground state.

We try now to get a good approximation for the elementary excitation by superposition of the $\psi_{ij}$. Define $\psi_c = \sum_{\langle i,j\rangle \in L} c_{ij} \psi_{ij}$, where $c = (c_{ij})_{\langle i,j\rangle \in L}$; then we want to choose $c$ in such a way that $\langle \psi_c | H | \psi_c \rangle / \langle \psi_c | \psi_c \rangle$ is minimized. We observe that $\langle \psi_{ij} | H | \psi_{kl} \rangle = 0$ for $\langle i, j\rangle \neq \langle k, l\rangle$, since $P_{mn} \psi_{ij} = 0$ or $P_{mn} \psi_{kl} = 0$ for all $\langle m, n\rangle$. Thus, we get

$$\frac{\langle \psi_c | H | \psi_c \rangle}{\langle \psi_c | \psi_c \rangle} = \frac{\sum_{\langle i,j\rangle} |c_{ij}|^2 \langle \psi_{ij} | H | \psi_{ij} \rangle}{\sum_{\langle i,j\rangle, \langle k,l\rangle} c_{ij}^* c_{kl} \langle \psi_{ij} | H | \psi_{kl} \rangle} \tag{3.3}$$

In the case of translation invariance the $\langle \psi_{ij} | H | \psi_{ij} \rangle$ are all the same and the expression in (3.3) is minimized if $c$ is the eigenvector to the largest eigenvalue of the matrix $M_{ij,kl} = \langle \psi_{ij} | H | \psi_{kl} \rangle$.

Let us now examine the spin-1 chain with $N$ sites and periodic boundary conditions in the limit $N \to \infty$. For that we need some integration rules. Using

$$|u_i v_j - v_i u_j|^2 = \frac{1}{2}(1 - \Omega_i \cdot \Omega_j) \tag{3.4}$$

$$\int_{S^2} d\Omega \, \Omega_1 \cdot \Omega = 0 \tag{3.5}$$

$$\int_{S^2} d\Omega (\Omega_1 \cdot \Omega)(\Omega \cdot \Omega_2) = \frac{1}{3} \Omega_1 \cdot \Omega_2 \tag{3.6}$$

where $\Omega_i = (\cos\theta_i \sin\phi_i, \sin\theta_i \sin\phi_i, \cos\phi_i)$, it follows that

$$\begin{aligned}
&\int \prod_{k=i}^{j-1} |u_k v_{k+1} - v_k u_{k+1}|^2 \prod_{l=i+1}^{j-1} d\Omega_l \\
&\quad = \frac{1}{2^{j-i}} \int \prod_{k=i}^{j-1} (1 - \Omega_k \cdot \Omega_{k+1}) \prod_{l=i+1}^{j-1} d\Omega_l \\
&\quad = \frac{1}{2^{j-i}} \left[ 1 - \left( -\frac{1}{3} \right)^{j-i-1} \Omega_i \cdot \Omega_j \right]
\end{aligned} \tag{3.7}$$

The first thing we shall calculate is

$$\langle \psi_{i,i+1} | H | \psi_{i,i+1} \rangle = \langle \psi_{i,i+1} | P_{i,i+1} | \psi_{i,i+1} \rangle = \| P_{i,i+1} \psi_{i,i+1} \|^2$$

We shall set $\alpha = 1$, $\beta = 0$. Then, according to (1.8), we obtain

$$\begin{aligned}
&P_{i,i+1}(u_{i-1}v_i - v_{i-1}u_i)\, u_i u_{i+1} (u_{i+1}v_{i+2} - v_{i+1}u_{i+2}) \\
&\quad = \frac{1}{2} u_{i-1}(u_i^2 u_{i+1} v_{i+1} + u_i v_i u_{i+1}^2) v_{i+2} - v_{i-1} u_i^2 u_{i+1}^2 v_{i+2} \\
&\qquad - \frac{1}{6} u_{i-1}(u_i^2 v_{i+1}^2 + 4 u_i v_i u_{i+1} v_{i+1} + v_i^2 u_{i+1}^2) u_{i+2} \\
&\qquad + \frac{1}{2} v_{i-1}(u_i^2 u_{i+1} v_{i+1} + u_i v_i u_{i+1}^2) u_{i+2} \\
&\quad =: X(\Omega_{i-1}, \ldots, \Omega_{i+2})
\end{aligned} \tag{3.8}$$

By integration over $d\Omega_{i+3}, d\Omega_{i+4}, \ldots, d\Omega_{i-2}$ we get

$$\begin{aligned}
\| P_{i,i+1} \psi_{i,i+1} \|^2 = &\int d\Omega_{i-1} \cdots d\Omega_{i+2} \, |X(\Omega_{i-1}, \ldots, \Omega_{i+2}|^2 \\
&\times \frac{1}{2^{N-3}} \left[ 1 - \left( -\frac{1}{3} \right)^{N-4} \Omega_{i-1} \Omega_{i+2} \right]
\end{aligned} \tag{3.9}$$

Since $(-1/3)^{N-4}$ decreases exponentially for $N \to \infty$, we can neglect this term and get

$$\begin{aligned}
&\| P_{i,i+1} \psi_{i,i+1} \|^2 \\
&\quad = \int d\Omega_{i-1} \cdots d\Omega_{i+2} \, |X(\Omega_{i-1}, \ldots, \Omega_{i+2}|^2 \\
&\quad = \left( \frac{1}{4} 2 \frac{1}{2} \cdot \frac{1}{3} \cdot \frac{1}{6} \cdot \frac{1}{2} + \frac{1}{2} \cdot \frac{1}{3} \cdot \frac{1}{3} \cdot \frac{1}{2} + \frac{1}{36} \cdot \frac{1}{2} \left( \frac{1}{3} \cdot \frac{1}{3} + 16 \frac{1}{6} \cdot \frac{1}{6} + \frac{1}{3} \cdot \frac{1}{3} \right) \cdot \frac{1}{2} \right. \\
&\qquad \left. + \frac{1}{4} 2 \frac{1}{2} \cdot \frac{1}{3} \cdot \frac{1}{6} \cdot \frac{1}{2} \right) \frac{1}{2^{N-3}} = \frac{5}{56} \frac{1}{2^{N-2}}
\end{aligned} \tag{3.10}$$

Next we calculate $\langle\psi_{i,i+1}|\psi_{i,i+1}\rangle$. By integration over $d\Omega_{i+2}$, $d\Omega_{i+3}$,..., $d\Omega_{i-1}$ we get

$$\langle\psi_{i,i+1}|\psi_{i,i+1}\rangle=\frac{1}{2^{N-1}}\int|u_i|^2|u_{i+1}|^2\left[1-\left(-\frac{1}{3}\right)^{N-2}\Omega_i\cdot\Omega_{i+1}\right]d\Omega_i\,d\Omega_{i+1} \tag{3.11}$$

Again we can neglect $(-1/3)^{N-2}$ and obtain

$$\langle\psi_{i,i+1}|\psi_{i,i+1}\rangle=\frac{1}{2^{N-1}}\frac{1}{4} \tag{3.12}$$

Similarly we get for $\langle\psi_{i,i+1}|\psi_{i+1,i+2}\rangle$

$$\begin{aligned}\langle\psi_{i,i+1}|\psi_{i+1,i+2}\rangle&\\ &=\frac{1}{2^{N-2}}\int u_i^*u_{i+1}^*(u_{i+1}v_{i+2}-v_{i+1}u_{i+2})^*u_{i+1}u_{i+2}\\ &\quad\times(u_iv_{i+1}-v_iu_{i+1})\,d\Omega_i\,d\Omega_{i+1}\,d\Omega_{i+2} \qquad (3.13)\\ &=-\frac{1}{2^{N-2}}\int u_i^*u_{i+1}^*v_{i+1}^*u_{i+2}^*u_{i+1}u_{i+2}u_iv_{i+1}\,d\Omega_i\,d\Omega_{i+1}\,d\Omega_{i+2}\\ &=-\frac{1}{2^{N-2}}\cdot\frac{1}{2}\cdot\frac{1}{6}\cdot\frac{1}{2}=-\frac{1}{2^{N-2}}\frac{1}{24} \qquad (3.14)\end{aligned}$$

It remains to calculate $\langle\psi_{i,i+1}|\psi_{i+n,i+n+1}\rangle$ for $n\geqslant 2$.

After integration over all sites but $i$, $i+1$, $i+n$, and $i+n+1$, we obtain, using (3.4),

$$\begin{aligned}\langle\psi_{i,i+1}|\psi_{i+n,i+n+1}\rangle&\\ &=\frac{1}{2^{N-2}}\int u_i^*u_{i+1}^*(u_{i+n}v_{i+n+1}-v_{i+n}u_{i+n+1})^*\\ &\quad\times u_{i+n}u_{i+n+1}(u_iv_{i+1}-v_iu_{i+1})\left[1-\left(-\frac{1}{3}\right)^{n-2}\Omega_{i+1}\Omega_{i+n}\right]\\ &\quad\times d\Omega_i\,d\Omega_{i+1}\,d\Omega_{i+n}\,d\Omega_{i+n+1} \qquad (3.15)\\ &=\frac{1}{2^{N-2}}\left[1-\left(-\frac{1}{3}\right)^{n-2}\right]\int u_i^*u_{i+1}^*u_{i+n}^*v_{i+n+1}^*u_{i+n}u_{i+n+1}u_iv_{i+n}\\ &\quad\times d\Omega_i\,d\Omega_{i+1}\,d\Omega_{i+n}\,d\Omega_{i+n+1} \qquad (3.16)\\ &\quad+\frac{1}{2^{N-2}}2\left(-\frac{1}{3}\right)^{n-2}\int u_i^*u_{i+1}^*(u_{i+n}v_{i+n+1}=v_{i+n}u_{i+n+1})^*\\ &\quad\times u_{i+n}u_{i+n+1}(u_iv_{i+1}-v_iu_{i+1}|u_{i+1}v_{i+n}-v_{i+1}u_{i+n}|^2\\ &\quad\times d\Omega_i\,d\Omega_{i+1}\,d\Omega_{i+1}\,d\Omega_{i+n+1} \qquad (3.17)\end{aligned}$$

$$= \frac{1}{2^{N-3}} \left(-\frac{1}{3}\right)^{n-2} \int u_i^* u_{i+1}^* v_{i+n}^* u_{i+n+1}^* u_{i+n} u_{i+n+1} u_i v_{i+1}$$

$$\times u_{i+1} v_{i+n} v_{i+1}^* u_{i+n}^* \, d\Omega_i \, d\Omega_{i+1} \, d\Omega_{i+n} \, d\Omega_{i+n+1} \quad [\text{since } (3.16) = 0] \tag{3.18}$$

$$= \frac{1}{2^{N-3}} \left(-\frac{1}{3}\right)^{n-2} \frac{1}{2} \cdot \frac{1}{6} \cdot \frac{1}{6} \cdot \frac{1}{2} = \frac{1}{2^{N-2}} \frac{1}{8} \left(-\frac{1}{3}\right)^n \tag{3.19}$$

Looking at (3.12) and (3.14), we see that (3.19) is also valid for $n = 0$ and $n = 1$. We must now calculate the highest eigenvalue of the matrix $M_{ij} = (-1/3)^{|i-j|}$, $i, j \in \mathbf{Z}$. That is an easy task. The corresponding eigenvector is $c_i = (-1)^i$ $(i \in \mathbf{Z})$, and from

$$\sum_{j \in \mathbf{Z}} M_{ij} c_j = c_i + (-1)^i \sum_{j=i+n}^{\infty} \left(\frac{1}{3}\right)^{j-i} + (-1)^i \sum_{j=-\infty}^{i-1} \left(\frac{1}{3}\right)^{i-j} = 2c_i \tag{3.20}$$

it follows that the highest eigenvalue is 2. We get for the energy gap $\varepsilon$ therefore the upper bound

$$\varepsilon \leqslant \frac{5}{56} \frac{8}{2} = \frac{5}{14} = 0.3\overline{571428} \tag{3.21}$$

and we have proven the following.

**Table I. Spin-1 Chain with Free Boundary Conditions**

| Number of sites | Eigenvalue of first excited state | Total spin |
|---|---|---|
| 3 | 0.5 | 2 |
| 4 | 0.448956 | 2 |
| 5 | 0.413240 | 2 |
| 6 | 0.398451 | 2 |

**Table II. Spin-1 Chain with Periodic Boundary Conditions**

| Number of sites | Eigenvalue of first excited state | Total spin |
|---|---|---|
| 4 | 0.333333 | 1 |
| 5 | 0.453957 | 1 |
| 6 | 0.347866 | 1 |

**Table III. Chain of Four Sites with Free Boundary Conditions for Higher Spins per Site**

| Spin per site | Eigenvalue of first excited state | Total spin |
|---|---|---|
| 1 | 0.448956 | 2 |
| 3/2 | 0.427345 | 4 |
| 2 | 0.418759 | 6 |
| 5/2 | 0.414143 | 8 |

**Table IV. Lattices in Figs. 1 and 2 with Spin 3/2 per Site**

| Lattice | Spin per site | Eigenvalue of first excited states | Total spin |
|---|---|---|---|
| Fig. 1 | 3/2 | 0.180196 | 4 |
| Fig. 2 | 3/2 | 0.7 | 1 |

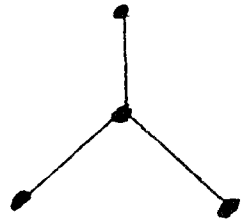

Fig. 1. Sublattice of the hexagonal lattice containing four sites.

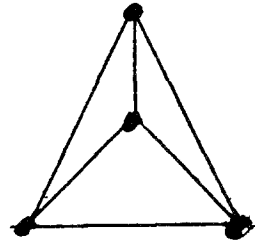

Fig. 2. The same lattice as in Fig. 1, but with closed boundary conditions. The coordination number at each site is 3.

**Theorem 3.1.** Let $\varepsilon_{1,N}$ be the energy gap of $H_{S,N}$ with spin $S=1$. Then

$$\overline{\lim_{N\to\infty}}\ \varepsilon_{1,N} \leqslant 5/14 \tag{3.22}$$

Comparing this result with the numerical values in Table II, we see that this upper bound is very good. The value for five sites is much higher than the values for an even number of sites. The reason is some kind of frustration: We have seen that the best superposition of the crackion is the one with alternating signs. But this is impossible for an odd number of sites.

If we look at the numerical results with free boundary conditions in Tables I, III, and IV, we see that in these cases in the first exicted state the free spins and the spin 1 of the crackion together form the highest possible total spin. For the hexagonal and the square lattice one can show by random walk technique as in ref. 2 that

$$\langle \psi_{ij} | \psi_{kl} \rangle / \langle \psi_{ij} | \psi_{ij} \rangle \tag{3.23}$$

decays exponentially with the distance of the links $\langle i, j \rangle$ and $\langle k, l \rangle$. Therefore these terms are the matrix elements of a bounded operator with finite highest eigenvalue. Thus we get an energy gap at least in the crackion approximation.

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