# AN ANALYSIS OF THE SPIN <br> WAVE APPROXIMATION FOR THE SPIN $\frac{1}{2}$ ANTIFERROMAGNET* 

David Kung<br>Stanford Linear Accelerator Center<br>Stanford University, Stanford, California, 94905


#### Abstract

A calculation has been done on the one and two dimension Heisenberg antiferromagnet in an alternating field to extract the external field critical exponent. The results obtained by the Projector Monte Carlo Method on finite lattices are extrapolated to the infinite volume limit using finite size scaling. The exponents are calculated to be 0.62 and 0.69 in one and two dimensions respectively, contradicting the estimate ( 0.5 in any dimension) predicted by the spin-wave approximation.


## Submitted to Physical Review B

[^0]
## 1. INTRODUCTION

The Heisenberg antiferromagnet has been studied extensively as a model for magnetism in the past several decades. Apart from the thermodynamics of the model, the energy spectrum of the Heisenberg antiferromagnet at zero temperature has also been investigated. The eigenvalue problem at zero field in 1 dimension has been solved by Bethe ${ }^{1}$ and the eigenvalues of the ground and low-lying excited states were also obtained in closed form ${ }^{2}$. In higher dimensions and for a general spin s no exact solutions have been obtained, so various approximations have to be made.

In one approach, the spin operators of the antiferromagnet are mapped onto bosonic spin wave variables and there exists a direct relationship between the matrix elements of the spin Hamiltonian and its bosonic counterpart, provided that the bosonic operator is projected onto an appropriate subspace. An approximation scheme, henceforth referred to as the spin wave approximation ${ }^{3}$, is to neglect terms higher than quadratic in the boson operator and work in the full boson space. The resulting approximate boson Hamiltonian, $H^{\text {trun }}$, indeed reproduces certain qualitative features of the original spin Hamiltonian, $H^{\text {spin }}$, such as the existence of massless spin waves which become massive when an external field is turned on. Anderson ${ }^{3}$ also has shown that the lowest eigenvalues of $H^{\text {trun }}$ and $H^{\text {spin }}$ for the spin $\frac{1}{2}$ case agree to within a few percent in both one and two dimensions. However, the spin wave approximation is justified only when the spin operators are in an infinite dimensional representation, and should fail in one dimension due to infrared divergences. Moreover, for spin $\frac{1}{2}, H^{\text {trun }}$ cannot be viewed as a lowest order approximation to $H^{\text {spin }}$ in which terms left out are manifestly small so that they can be treated as a negligible perturbation. In view
of these facts, the good agreement in the ground state energy values is probably accidental.

To investigate whether $H^{\text {trun }}$ is actually a good approximation to $H^{\text {spin }}$ for the spin $\frac{1}{2}$ case, we have to compare quantities which are more sensitive to approximations than the ground state energy. In the presence of an external alternating field $\epsilon$, the spin wave approximation predicts a mass gap proportional to $\epsilon^{\frac{1}{2}}$. In this paper we treat $H^{\text {spin }}$ as an eigenvalue problem and calculate numerically the mass of the spin wave state as a function of $\epsilon$ for finite systems. Then we use finite size scaling ${ }^{6}$ to extract the exponent $\nu$, where $m_{\text {spin wave }} \propto \epsilon^{\nu}$, which will be compared with the value predicted by the spin wave approximation. In section II the boson mapping is reviewed and we attempt to explain the good agreement between the ground state energies of $H^{\text {spin }}$ and $H^{\text {trun }}$. The computational method ${ }^{5}$, the projector Monte Carlo, is presented in section III. We will employ finite size scaling technique, which is described in section IV, to extract information about the infinite volume limit and we discuss our results in section V.

## 2. THE SPIN WAVE APPROXIMATION

### 2.1 The Boson Mapping ${ }^{8}$

We will describe the boson mapping for an arbitrary spin $s$ and then restrict to the spin $\frac{1}{2}$ case. In a spin $\mathrm{S} S U(2)$ antiferromagnet the spin variables satisfy the commutation relations

$$
\begin{equation*}
\left[s_{z}, s_{ \pm}\right]= \pm s_{ \pm}, \quad\left[s_{+}, s_{-}\right]=2 s_{z} \tag{2.1}
\end{equation*}
$$

Let us define the following operators

$$
\begin{align*}
& \tilde{s}_{+}=\sqrt{2 s} a^{\dagger} \\
& \tilde{s}_{-}=\sqrt{2 s}\left(1-\frac{1}{2 s} a^{\dagger} a\right) a  \tag{2.2}\\
& \widetilde{s}_{z}=-s+a^{\dagger} a
\end{align*}
$$

where the $a$ 's and $a^{\dagger}$ 's are the boson annihilation and creation operators satisfying

$$
\begin{equation*}
\left[a, a^{\dagger}\right]=1, \quad[a, a]=\left[a^{\dagger}, a^{\dagger}\right]=0 . \tag{2.3}
\end{equation*}
$$

It is straightforward to show that the $\widehat{s}$ 's satisfy the same commutation relations as in (2.1). The eigenvalues of $\widetilde{s}_{z}$ are $-s,-s+1 \ldots$ and have no upper bound while those of $s_{z}$ are $-s,-s+1 \ldots s-1, s$, hence the two kinds of operators act on different Hilbert spaces and are not equivalent. Nevertheless, we can still relate the matrix elements of $s_{z}$ to those of $\tilde{s}_{z}$. Let us begin by building up the Hilbert space, $H_{1}$, of the $\hat{\mathcal{s}}$ 's in the occupation number representation. We start with the base state $\phi_{0}$ with the property

$$
\begin{equation*}
a \phi_{0}=0 \tag{2.4}
\end{equation*}
$$

and the rest of the states are defined as

$$
\begin{equation*}
\phi_{n}=\frac{1}{\sqrt{n!}}\left(a^{\dagger}\right)^{n} \phi_{n} \tag{2.5}
\end{equation*}
$$

so that

$$
\begin{equation*}
a^{\dagger} a \phi_{n}=n \phi_{n} \tag{2.6}
\end{equation*}
$$

and the inner product is defined as

$$
\begin{equation*}
\left(\phi_{n}, \phi_{n^{\prime}}\right)=\delta_{n n^{\prime}} . \tag{2.7}
\end{equation*}
$$

We will denote the states with $\mathrm{n} \leq 2 s$ physical and states with $n>2 s$ unphysical. With the above metric for the inner product $\widetilde{s}_{+}$is not the Hermitian conjugate of $\widetilde{s}_{-}$. Requiring that $\widetilde{s}_{+}$be the Hermitian conjugate of $\widetilde{s}_{-}$and that $\widetilde{s}_{z}$ be self-adjoint uniquely define an indefinite metric, $F$, which is diagonal in the occupation number representation and has the property

$$
\begin{equation*}
F_{n}=\left(\phi_{n}, F \phi_{n}\right) ; \quad F_{n}=1 \cdot\left(1-\frac{1}{2 s}\right) \cdots\left(1-\frac{n-1}{2 s}\right) . \tag{2.8}
\end{equation*}
$$

With this metric for the inner product,

$$
\begin{equation*}
\left\langle\phi_{n}, \phi_{n^{\prime}}\right\rangle \equiv\left(\phi_{n}, F \phi_{n^{\prime}}\right)=F_{n} \delta_{n n^{\prime}}, \tag{2.9}
\end{equation*}
$$

the unphysical states have zero norms.
The Hilbert space, $H_{2}$, of the $s$ 's are built starting with the state $|0\rangle$ defined by

$$
\begin{equation*}
s_{-}|0\rangle=0, \quad s_{z}|0\rangle=-s|0\rangle \tag{2.10}
\end{equation*}
$$

and the rest are obtained by raising on $|0\rangle$

$$
\begin{equation*}
|n\rangle=\frac{1}{(\sqrt{2 s})^{n}} \frac{1}{\sqrt{n!}}\left(s_{+}\right)^{n}|0\rangle \tag{2.11}
\end{equation*}
$$

so that

$$
\begin{equation*}
s_{z}|n\rangle=(n-s)|n\rangle \tag{2.12}
\end{equation*}
$$

These states are orthogonal but not normalized

$$
\begin{equation*}
\left\langle n \mid n^{\prime}\right\rangle=F_{n} \delta_{n n^{\prime}} \tag{2.13}
\end{equation*}
$$

where $F_{n}$ is given by (2.8).
We now quote the main result that relates the matrix elements of $s$ to those of $\widetilde{s}$ : if $G(s)$ is an arbitrary function of spin operators $s$, then

$$
\begin{equation*}
\langle n| G(s)\left|n^{\prime}\right\rangle=\left(\phi_{n}, F G(P \widetilde{s} P) \phi_{n^{\prime}}\right) \tag{2.14}
\end{equation*}
$$

where $P_{j}$ is the projection operator onto the subspace of physical states of $H_{1}$ :

$$
P \phi_{n}=\left\{\begin{array}{cc}
\phi_{n} & n \leq 2 s  \tag{2.15}\\
0 & n>2 s
\end{array}\right.
$$

### 2.2 The Truncated Hamiltonian

We proceed to apply the boson mapping to the spin Hamiltonian

$$
\begin{equation*}
H^{\mathrm{spin}}=\sum_{\langle j, \ell\rangle} \frac{1}{2}\left(s_{j}^{A_{+}} s_{\ell}^{B_{-}}+s_{j}^{A_{-}} s_{\ell}^{B_{+}}\right)+g s_{j}^{A_{z}} s_{\ell}^{B_{x}}-\epsilon\left(\sum_{j} s_{j}^{A_{z}}-\sum_{l} s_{l}^{B_{z}}\right) \tag{2.16}
\end{equation*}
$$

where $\langle j, \ell\rangle$ denotes the sum over nearest neighbors, $A$ and $B$ refer to two interlocking $d$-dimensional hypercubical sublattices, with $N$ sites in each, and the $s$ 's are in the spin $s$ representation of $\mathrm{SU}(2)$. The quantization axes of the two sublattices are rotated 180 degrees with respect to each other so that

$$
\begin{array}{ll}
s_{j}^{A_{+}}\left|0_{j}\right\rangle=0, & s_{\ell}^{B_{-}}\left|0_{\ell}\right\rangle=0, \\
s_{j}^{A_{x}}\left|0_{j}\right\rangle=s\left|0_{j}\right\rangle, & s_{\ell}^{B_{z}}\left|0_{\ell}\right\rangle=-s\left|0_{\ell}\right\rangle . \tag{2.17}
\end{array}
$$

With this rotation, the Dyson-Maleev ${ }^{4}$ transformation on this two-sublattice
model is

$$
\begin{array}{ll}
s_{j}^{A_{+}} \rightarrow \sqrt{2 s}\left(1-a_{j}^{\dagger} a_{j}\right) a_{j} & s_{\ell}^{B_{+}} \rightarrow \sqrt{2 s} b_{\ell}^{\dagger} \\
s_{j}^{A_{-}} \rightarrow \sqrt{2 s} a_{j}^{\dagger} & s_{\ell}^{B_{-}} \rightarrow \sqrt{2 s}\left(1-\frac{b_{\ell}^{\dagger} b_{\ell}}{2 s}\right) b_{\ell}  \tag{2.18}\\
s_{j}^{A_{z}} \rightarrow+s-a_{j}^{\dagger} a_{j} & s^{B_{z}} \rightarrow-s+b_{\ell}^{\dagger} b_{\ell} .
\end{array}
$$

The bosonized operator derived from $H^{\text {spin }}$ is

$$
\begin{align*}
\tilde{H}= & -g N s^{2} z-2 N \epsilon s+\sum_{\langle j, \ell\rangle} s\left(\left(1-\frac{a_{j}^{\dagger} a_{j}}{2 s}\right) a_{j}\left(1-\frac{b_{\ell}^{\dagger} b_{\ell}}{2 s}\right) b_{\ell}+a_{j}^{\dagger} b_{\ell}^{\dagger}\right)  \tag{2.19}\\
& +(g s z+\epsilon)\left(\sum_{j} a_{j}^{\dagger} a_{j}+\sum_{\ell} b_{\ell}^{\dagger} b_{\ell}\right)-g \sum_{\langle j, \ell\rangle} a_{j}^{\dagger} a_{j} b_{\ell}^{\dagger} b_{\ell}
\end{align*}
$$

where $z=2 d$.
The spin wave approximation consists of approximating $H^{\text {spin }}$ by

$$
\begin{align*}
H^{\text {trun }}= & -g s^{2} N z-2 N \epsilon s+\sum_{\langle j, \ell\rangle} s\left(a_{j} b_{j}+a_{j}^{\dagger} b_{\ell}^{\dagger}\right)  \tag{2.20}\\
& +(g s z+\epsilon)\left[\sum_{j} a_{j}^{\dagger} a_{j}+\sum_{\ell} b_{\ell}^{\dagger} b_{\ell}\right]
\end{align*}
$$

This approximation for the low-lying spectrum is justified for $s \rightarrow \infty$ for the following reasons. The spin space and the boson space will be matched up so the entire boson space is physical. Furthermore, the dominant configurations in the low-lying states do not deviate substantially from the mean-field configurations so that the terms omitted from $\tilde{H}$ are suppressed by $\frac{1}{s}$.

The advantage of working with $H^{\text {trun }}$ is that it can be solved exactly by first Fourier-transforming to momentum space:

$$
\begin{align*}
a_{j} & =\frac{1}{\sqrt{N}} \sum_{k} e^{i k j} a_{k}  \tag{2.21}\\
b_{\ell} & =\frac{1}{\sqrt{N}} \sum_{k} e^{-i k \ell} b_{k}
\end{align*}
$$

We obtain the following Hamiltonian

$$
\begin{align*}
H^{\text {trun }}= & -g s^{2} N z-2 N \epsilon s \\
& +\sum_{k}\left\{s z \gamma_{k}\left(a_{k}^{\dagger} b_{k}^{\dagger}+a_{k} b_{k}\right)+(g s z+\epsilon)\left[a_{k}^{\dagger} a_{k}+b_{k}^{\dagger} b_{k}\right]\right\} \tag{2.22}
\end{align*}
$$

where

$$
\begin{equation*}
\gamma_{k}=\frac{1}{z} \sum_{\delta} e^{i k \delta} \tag{2.23}
\end{equation*}
$$

This Hamiltonian can be diagonalized by the Bogoliubov transformation

$$
\begin{array}{r}
a_{k}=u_{k} \alpha_{k}+v_{k} \beta_{k}^{\dagger}  \tag{2.24}\\
b_{k}=u_{k} \beta_{k}+v_{k} \alpha_{k}^{\dagger}
\end{array}
$$

where the $u_{k}$ 's and $v_{k}$ 's are real and

$$
\begin{equation*}
u_{k}^{2}-v_{k}^{2}=1 \quad \text { for all } k \tag{2.25}
\end{equation*}
$$

to preserve the canonical commutation relations. Written in terms of the $\alpha$ 's and
$\beta$ 's

$$
\begin{equation*}
H^{\operatorname{trun}}=\sum_{k}\left(\alpha_{k}^{\dagger} \alpha_{k}+\beta_{k}^{\dagger} \beta_{k}\right) \omega_{k}-g(s+1) s N z-2 N \epsilon s-\epsilon N \tag{2.26}
\end{equation*}
$$

where

$$
\begin{equation*}
\omega_{k}=\sqrt{(g s z \epsilon)^{2}-\left(s z \gamma_{k}\right)^{2}} \tag{2.27}
\end{equation*}
$$

provided that

$$
\begin{equation*}
u_{k}=\left(\frac{1}{2}+\frac{g s z+\epsilon}{2 \omega_{k}}\right)^{1 / 2} \quad v_{k}=-\left(\frac{1}{2}-\frac{g s z+\epsilon}{2 \omega_{k}}\right)^{1 / 2} . \tag{2.28}
\end{equation*}
$$

The ground state, $\left|\Omega_{t}\right\rangle$, is the one annihilated by all the $\alpha_{k}$ 's and $\beta_{k}$ 's. From the dispersion relation we conclude that the mass of excitations created by the $\alpha^{\dagger}$ 's and $\beta^{\dagger}$ 's from the ground state is proportional to $\epsilon^{\frac{1}{2}}$.

In what follows we deal exclusively with the spin $\frac{1}{2}$ case, where there is maximal mismatch between the physical subspace and the full boson space. Moreover, $\frac{1}{s}$ is of order one so the terms omitted are not suppressed. Despite these facts, there have been arguments which suggest that the spin wave approximation may be better than it seems. The fact that $\left\langle\Omega_{t}\right| a_{j}^{\dagger} a_{j}\left|\Omega_{t}\right\rangle$ diverges in 1 dimension but is 0.078 in 2 dimensions has been used to indicate that the spin wave approximation may be reasonable in dimensions higher than two ${ }^{9}$. We will show that $\left\langle\Omega_{t}\right| a_{j}^{\dagger} a_{j}\left|\Omega_{t}\right\rangle \ll 1$ does not necessarily require $\left|\Omega_{t}\right\rangle$ to have a negligible unphysical component. As an example, let us consider the state

$$
|\phi\rangle=\frac{1}{2 \sqrt{N d}} \sum_{\langle j, \ell\rangle}\left(a_{j}^{\dagger}\right)^{2}\left(b_{\ell}^{\dagger}\right)^{2} \hat{\phi}_{0}
$$

where

$$
\begin{equation*}
\hat{\phi}_{0}=\Pi_{j} \Pi_{\ell} \phi_{0}(j) \phi_{0}(\ell) \tag{2.29}
\end{equation*}
$$

We see that $\langle\phi| a_{j}^{\dagger} a_{j}|\phi\rangle$ is infinitesimal although ${ }^{-}|\phi\rangle$ has no physical component. It is states such as these which will mix with the physical states to lowest order in $H^{\text {trun }}$.

Another argument in support of the spin wave approximation is that the ground state energy densities of $H^{\text {trun }}$ in one and two dimensions are -0.433 and -0.658 respectively, agreeing very well with the exact result of -0.443 in 1 dimension ${ }^{2}$ and the numerical estimate of -0.655 in 2 dimensions ${ }^{12}$. We can understand the good agreement between the ground state energies of $H^{\text {trun }}$ and $H^{\text {spin }}$ in the following way. We note that for spin $\frac{1}{2}$ the states $|n\rangle$ are normalized, therefore identifying $|n\rangle$ at each site with $\phi_{n}$ at the same site, we conclude from (2.14) that $H^{\text {spin }}$ and $\hat{P}_{\frac{1}{2}} \widetilde{H} \hat{P}_{\frac{1}{2}}$ have the same matrix elements, where

$$
\begin{equation*}
\hat{P}_{1 / 2}=\Pi_{j \in A} P_{1 / 2}(j) \Pi_{\ell \in B} P_{1 / 2}(\ell) \tag{2.30}
\end{equation*}
$$

$H^{\text {trun }}$ can be written as

$$
H^{\text {trun }}=\left[\begin{array}{lr}
\hat{H} & M  \tag{2.31}\\
M & X
\end{array}\right]
$$

where

$$
\begin{equation*}
\hat{H}=\hat{P}_{1 / 2} H^{\mathrm{trun}} \hat{P}_{1 / 2}=H^{\mathrm{spin}}+g \hat{P}_{1 / 2} \sum_{\langle j, \ell\rangle} a_{j}^{\dagger} a_{j} b_{\ell}^{\dagger} b_{\ell} \hat{P}_{1 / 2} . \tag{2.32}
\end{equation*}
$$

$M$ is an operator which connects unphysical states to physical states and $X$ is an operator in the unphysical sector. If we denote the ground state energies of $H^{\text {spin }}, H^{\text {trun }}$, and $\hat{H}$ by $E^{\text {spin }}, E^{\text {trun }}$, and $\hat{E}$ respectively, then Eq. (2.32) implies that

$$
\begin{equation*}
\hat{E}=E^{\mathrm{spin}}+\Delta_{1} \quad \Delta_{1}>0 \tag{2.33}
\end{equation*}
$$

because the $a_{j}^{\dagger} a_{j} b_{l}^{\dagger} b_{l}$ terms are diagonal and manifestly positive. From (2.31), it
is clear that mixing between physical and unphysical states lowers the ground state energy of $\hat{H}$ so that

$$
\begin{equation*}
E^{\text {trun }}=\hat{E}-\Delta_{2} \quad \Delta_{2}>0 \tag{2.34}
\end{equation*}
$$

Combining Eqs. (2.33) and (2.34) we obtain

$$
\begin{equation*}
E^{\text {trun }}=E^{\mathrm{spin}}+\Delta_{1}-\Delta_{2} \tag{2.35}
\end{equation*}
$$

so that the close agreement of the ground state energies arises from a fortuitous cancellation of errors originating from two unrelated sources.

This good agreement can well be accidental since it is not uncommon for a poor trial state to yield a good ground state energy estimate. In one dimension, $\Delta_{1}=0.058$ and $\Delta_{1}-\Delta_{2}=0.007$, so both $\Delta$ 's are sizable relative to $E^{\text {spin }}$. This suggests that $\left|\Omega_{t}\right\rangle$ differs significantly from the ground state of $H^{\text {spin }}$ unless there is yet another miraculous cancellation. To pursue these matters quantitatively, we numerically calculate the exponent $\nu$ for $H^{\text {spin }}$ and compare it with the predicted value of $H^{\text {trun }}$. If the two values of $\nu$ differ substantially, then it is unlikely that $H^{\text {trun }}$ is a good approximation to $H^{\text {spin }}$. In the following section we will present the numerical technique required for such a calculation.

## 3. Numerical Method

The quantity we are interested in computing is the difference between the ground state of $H^{\text {spin }}$ and the zero momentum spin wave state, for a given external field strength $\epsilon$. The operator $Q_{z}=\sum_{i} s_{z}^{i}$ commutes with $H^{\text {spin }}$, so we can classify states according to the quantum number $Q_{z}$. The ground state is lowestlying in the $Q_{z}=0$ sector and the spin wave approximation suggests that the zero-momentum spin wave states are lowest-lying in the degenerate $Q_{z}= \pm 1$ sector.

With a conserved quantum number at our disposal, we can choose a specific $|\phi\rangle$ in the $Q_{z}=0,1$ sector and use the projection operator $\lim _{\beta \rightarrow \infty} e^{-\beta H^{\text {spin }}}$ to project onto the lowest energy eigenstate in the respective $Q_{z}=0,1$ sector. Following Blankenbecler et al. ${ }^{5}$, we consider the equation

$$
\begin{equation*}
E=-\lim _{\beta \rightarrow \infty} \frac{1}{\Delta \beta} \ln \frac{\langle\chi| e^{-(\beta+\Delta \beta) H^{\mathrm{spin}}}|\phi\rangle}{\left\langle\chi e^{-\beta H^{\mathrm{spin}}} \mid \phi\right\rangle}, \tag{3.1}
\end{equation*}
$$

in which $E$ is the lowest energy eigenvalue of $H^{\text {spin }}$ in the $Q_{z}=0\left(Q_{z}=1\right)$ sector if both $|\phi\rangle$ and $|\chi\rangle$ belong to the $Q_{z}=0\left(Q_{z}=1\right)$ sector. The problem now reduces to the evaluation of the matrix element $\langle\chi| e^{-\beta H^{\text {spin }}}|\phi\rangle$.

To evaluate $\langle\chi| e^{-\beta H^{\text {spin }}}|\phi\rangle$, we first define

$$
\begin{equation*}
U=e^{-\Delta \tau H^{\text {spin }}} \tag{3.2}
\end{equation*}
$$

where

$$
\Delta \tau=\frac{\beta}{N}
$$

so that

$$
\begin{equation*}
e^{-\beta H^{\mathrm{spin}}}=U^{N} \tag{3.3}
\end{equation*}
$$

Then we decompose $H^{\text {spin }}$ into

$$
\begin{equation*}
H^{\mathrm{spin}}=H_{1}+H_{2} \tag{3.4}
\end{equation*}
$$

such that the matrix elements of the operators

$$
\begin{equation*}
U(k)=e^{-\Delta \tau H_{k}} \quad k=1,2 \tag{3.5}
\end{equation*}
$$

are easy to evaluate. In this way,

$$
\begin{equation*}
U=U(2) U(1)+\theta\left(\Delta \tau^{2}\right) \tag{3.6}
\end{equation*}
$$

For our one dimensional problem, the decomposition is

$$
\begin{align*}
& H_{1}=\sum_{i \text { odd }}-\frac{1}{2}\left(s_{i}^{+} s_{i+1}^{-}+s_{i}^{-} s_{i+1}^{+}\right)+s_{i}^{z} s_{i+1}^{z}+\frac{\epsilon}{2}\left(-s_{i}^{z}+s_{i+1}^{z}\right) \\
& H_{2}=\sum_{i \text { even }}-\frac{1}{2}\left(s_{i}^{+} s_{i+1}^{-}+s_{i}^{-} s_{i+1}^{+}\right)+s_{i}^{z} s_{i+1}^{z}-\frac{\epsilon}{2}\left(-s_{i}^{z}+s_{i+1}^{z}\right) \tag{3.7}
\end{align*}
$$

Periodic boundary condition is imposed on the finite systems and the generalization to two dimensions is obvious. Hence

$$
\begin{align*}
Y(\beta) & \equiv\langle\chi| e^{-\beta H^{\mathrm{spin}}}|\phi\rangle \\
& \simeq\langle\chi|[U(2) U(1)]^{N}|\phi\rangle  \tag{3.8}\\
& =\sum_{i_{2 N+1}, \ldots i_{1}}\left\langle\chi \mid i_{2 N+1}\right\rangle\left\langle i_{2 N+1}\right| U(2)\left|i_{2 N}\right\rangle \ldots\left\langle i_{2}\right| U(1)\left|i_{1}\right\rangle\left\langle i_{1} \mid \phi\right\rangle .
\end{align*}
$$

The sum over intermediate states is performed by Monte Carlo with importance sampling. We write

$$
\begin{equation*}
\langle i| U(k)|j\rangle=P_{i j}(k) S_{i j}(k) \quad k=1,2 \tag{3.9}
\end{equation*}
$$

with the condition that the $P(k)$ 's are positive semi-definite and $\sum_{i} P_{i j}(k)=1$ for all $j$ 's and $k=1,2$. The procedure for evaluating $Y(\beta)$ is as follows. We choose a specific state $\left|i_{1}\right\rangle$ with probability proportional to $\left|\left\langle\phi \mid i_{1}\right\rangle\right|$. Then we choose a state $\left|i_{1}\right\rangle$ with probability $P_{i_{2} i_{1}}(1)$ and a state $\left|i_{3}\right\rangle$ with probability $P_{i_{3} i_{2}}(2)$ and so on. Having thus generated a $2 N+1$-tuple

$$
\begin{equation*}
\vec{i}(\beta)=\left(i_{1}, i_{2}, \ldots i_{2 N+1}\right) \tag{3.10}
\end{equation*}
$$

we assign to it a weight

$$
\begin{equation*}
w(\vec{i}(\beta), \phi, \chi)=\left\langle\chi \mid i_{2 N+1}\right\rangle S_{i_{2 N+1}, i_{2 N}}(2) \ldots . . . S_{i_{2}, i_{1}}(1)_{\zeta}, \tag{3.11}
\end{equation*}
$$

where $\varsigma=\operatorname{sgn}\left(\left\langle i_{1} \mid \phi\right\rangle\right)$. Each such configuration of intermediate states $\vec{i}_{\alpha}(\beta)$ is referred to as a random walk. This procedure is repeated $M$ times and we obtain

$$
\begin{equation*}
\frac{Y\left(\beta^{\prime}\right)}{Y(\beta)}=\lim _{M \rightarrow \infty} \frac{\sum_{\alpha=1}^{M} w\left(\vec{i}_{\alpha}\left(\beta^{\prime}\right), \phi, \chi\right)}{\sum_{\alpha=1}^{M} w\left(\vec{i}_{\alpha}(\beta), \phi, \chi\right)} \tag{3.12}
\end{equation*}
$$

where $\Delta \tau=\frac{\beta^{\prime}}{N^{\prime}}=\frac{\beta}{N}$.
The systematic errors due to the finiteness of $\Delta \tau$ and $\beta$, and various techniques to improve convergence of the Projector Monte Carlo are discussed extensively in a forthcoming paper. ${ }^{7}$

## 4. Finite Size Scaling

To extract information about the infinite volume limit, we favor using finite size scaling ${ }^{6}$ on small lattices over direct calculation on a large lattice because fluctuations increase while the mass gap decreases for increasing lattice size.

In the vicinity of the critical point of an infinite system, the system loses its fine-grained structure so that the correlation length sets the scale for all the dimensionful physical variables. This is the basis for the derivation of the scaling relations. Consider the corresponding situation of a finite system with a large enough linear dimension $L$ so that it exhibits pseudo-critical behavior. We assume that there are two dominant scales in this case, namely L and $\xi_{\infty}$, the infinite volume correlation length. To be more precise, finite size scaling states that the mass gap, $m_{L}(\kappa)$, in this finite system satisfies

$$
\begin{equation*}
m_{L}(\kappa)=\frac{1}{L} F_{L}\left(\frac{L}{\xi_{\infty}(\kappa)}\right) \tag{4.1}
\end{equation*}
$$

where $\kappa=g-g_{c}, g_{c}$ is the critical coupling and $F$ is an analytic function of $\kappa$.
Applying the above analysis to our Hamiltonian $H^{\text {spin }}$ on a finite lattice, the mass gap attains a minimum at $\epsilon=0$ because $m_{L}(\epsilon)$ is an even function of $\epsilon$. Hence, the critical coupling is at $\epsilon=0$, in which case $\kappa$ coincides with $\epsilon$. Assuming a power law singularity for the infinite volume correlation length,

$$
\begin{equation*}
\xi_{\infty}(\epsilon) \propto \epsilon^{-\nu} \tag{4.2}
\end{equation*}
$$

we obtain

$$
\begin{equation*}
m_{L}(\epsilon)=\frac{1}{L} F_{L}\left(L \epsilon^{\nu}\right) ; \quad \text { for } \epsilon \rightarrow 0 \tag{4.3}
\end{equation*}
$$

The analyticity of $F_{L}$ as a function of $\epsilon$ requires it to be a function of $y \equiv L^{\frac{1}{\nu}} \epsilon$.

For $\epsilon \ll 1$ so that $y \ll 1$ we taylor expand $F$ to get

$$
\begin{equation*}
F_{L}(\epsilon)=a+b L^{2 / \nu} \epsilon^{2}+\mathcal{O}\left(\epsilon^{4}\right) \tag{4.4}
\end{equation*}
$$

leading to

$$
\begin{equation*}
\nu=2 \ln \left(\frac{L_{1}}{L_{2}}\right) / \ln \left(\frac{F_{L_{1}}^{\prime}(0)}{F_{L_{2}}^{\prime}(0)}\right) \tag{4.5}
\end{equation*}
$$

where

$$
\begin{equation*}
F^{\prime}(0)=\frac{\partial F(0)}{\partial\left(\epsilon^{2}\right)} \tag{4.6}
\end{equation*}
$$

From the relationship between mass gap and correlation length

$$
\begin{equation*}
m_{\text {gap }} \propto \xi_{\infty}^{-1} \tag{4.7}
\end{equation*}
$$

we arrive at

$$
\begin{equation*}
m_{\text {spin wave }} \propto \mathcal{C} \epsilon^{\nu} \tag{4.8}
\end{equation*}
$$

## 5. Results

The results are obtained by applying the finite size scaling method to 4,6 and 8 site nearest neighbor models in 1 dimension, and to $2 \times 2,4 \times 4$ and $6 \times 6$ site nearest neighbor models in 2 dimensions. The data for 4 and 6 sites in 1 dimension and those for $2 \times 2$ sites in 2 dimensions are obtained from computer diagonalization of the Hamiltonian and the rest are obtained by the Projector Monte Carlo method.

The results are tabulated in Tables I-II. The statistical fluctuation for the ground and spin wave state energies is about a few parts in a thousand, and that magnifies to about a few percents in the mass gap. In figs. 1 and 2, the curves fitting the data points, $F_{L}(\epsilon)$ vs. $\epsilon$ cross very close to $\epsilon=0$. Hence, we expect finite size corrections to be small and we fit the various $F_{L}(\epsilon)$ 's with

$$
\begin{equation*}
b_{0}^{L}+b_{1}^{L} \epsilon^{2}+b_{2}^{L} \epsilon^{4}+b_{3}^{L} \epsilon^{6} . \tag{5.1}
\end{equation*}
$$

The final results are

$$
\begin{align*}
& \nu=0.62 \quad \text { 1-dimension }  \tag{5.2}\\
& \nu=0.69 \quad \text { 2-dimension } .
\end{align*}
$$

It is difficult to put an error bar on $\nu$ from fitting such few data points but the chi-square analysis yields a confidence level of over $99 \%$ for all the fits. If we force the fit to produce a $\nu$ of 0.5 , the confidence level drops to $44 \%$ for the 1 dimensional case and $0.1 \%$ for the 2 dimensional case. From this, we conclude that $\nu$ is unlikely to be 0.5 , especially in the 2 dimensional case.

## 6. Conclusions

The above calculation shows that the value of $\nu$ for both the one and two dimensional models are bigger than 0.5 , the value predicted by the spin-wave approximation. The increasing trend of $\nu$ as a function of dimension suggests that it is unlikely for $\nu$ to drop to 0.5 in three dimensions. Our calculation thus shows certain deficiencies of the spin-wave approximation, although it is not the viewpoint of the author that the spin-wave picture is entirely wrong. The fact that the mass gap does not show any essential singular behavior (e.g. Kosterlitz-Thouless type) as a function of $\epsilon$ indicates that interacting spin waves is a reasonable qualitative description for the low energy dynamics of the Heisenberg antiferromagnet, modulo non-linear effects which alter the exponent $\nu$ from the predicted value of 0.5. However, we would like to emphasize that the common belief claiming that the spin wave scenario is adequate for spin $\frac{1}{2}$ in two spatial dimensions and above should be challenged. As a bonus, we also obtain information about the behavior of $\nu$ as a function of $g$ for the one dimensional case. The model in one dimension is exactly solvable ${ }^{13}$ at $\mathrm{g}=0$ and it can be shown that $\nu=1$. From our calculation $\nu=0.62$ at $\mathrm{g}=1$; hence by continuity, $\nu$ must vary with g for g in the interval $[0,1]$. Thus, violation of universality occurs in $\nu$ as well as in the exponent for the power-law fall-off ${ }^{11}$ for the correlation functions.

## ACKNOWLEDGEMENTS

The author would like to thank Helen Quinn and Dick Blankenbecler for useful conversations and patient guidance throughout the course of this work.

## REFERENCES

1. H. A. Bethe, Z. Physik 71, 205 (1931).
2. R. Orbach, Phys. Rev. 112, 309 (1958). J. des Cloizeaux and M. Gaudin, Journal of Math. Phys. 7, 1384 (1966).
3. P. W. Anderson, Phys. Rev. 86, 694 (1952).
4. F. J. Dyson, Phys. Rev. 102, 1217 (1956). S. V. Maleev JEPT 6, 776 (1958).
5. R. Blankenbecler and R. Sugar, Phys. Rev. D27, 1304 (1983).
6. M. E. Fisher in Critical Phenomena, Proc. Int'l School of Physics, 'Enrico Fermi', Varenna 1970, ed. M. S. Green (New York: Academic).
7. R. Blankenbecler, R. Sugar and D. Kung (to be published).
8. A. I. Akhiezer, V. G. Bar'yakhtar and S. V. Peleminskii, "Spin Waves" (North Holland), Chap. 8.
9. D. C. Herbert, Journal of Math. Phys. 10, 225, (1969).
10. J. Smit Nuc. Phys. B175 307 (1980).
11. A. Luther and I. Perchel, Phys. Rev. B12, 3908 (1975).
12. J. Oitma and D. D. Betts, Canadian J. of Phys. $\underline{56}$, 897 (1978).
13. E. Lieb, T. D. Schultz and D. C. Mattis, Ann. of Phys. 16, 407 (1961).

TABLE 1
$F_{L}$ vs. $\epsilon^{2}$ and the slope at $\epsilon^{2}=0$ for 4,6 and 8 sites in one dimension.

4 sites

| $\epsilon^{2}$ |  | L $\times$ gap |
| :---: | :---: | ---: |
| 0 |  | 4.0000 |
| 0.01 |  | 4.0845 |
| 0.02 |  | 4.1648 |
| 0.03 |  | 4.2417 |
| 0.04 |  | 4.3153 |
| 0.05 |  | 4.3861 |
|  | slope $=8.66$ |  |
|  |  |  |
|  |  |  |
| $\epsilon^{2}$ |  | sites |
| 0 |  | 4.108 |
| 0.01 |  | 4.397 |
| 0.02 |  | 4.648 |
| 0.03 |  | 4.872 |
| 0.04 |  | 5.073 |
| 0.05 |  | 5.258 |

$$
\text { slope }=30.9
$$

8 sites

| $\epsilon^{2}$ | $\mathrm{~L} \times$ gap |
| ---: | :---: |
| 0 | $4.29 \pm 0.16$ |
| 0.005 | $4.68 \pm 0.08$ |
| 0.01 | $4.91 \pm 0.13$ |
| 0.02 | $5.56 \pm 0.09$ |
| 0.03 | $5.87 \pm 0.04$ |
| 0.04 |  |
| 0.05 |  |
|  | slope $=81.2$ |

TABLE 2
$F_{L}$ vs. $\epsilon^{2}$ and the slope at $\epsilon^{2}=0$ for $2 \times$ $2,4 \times 4$ and $6 \times 6$ sites in two dimensions.
$2 \times 2$ sites

| $\epsilon^{2}$ | $\mathrm{~L} \times \mathrm{gap}$ |  |
| :---: | ---: | ---: |
| 0 | 2.000 |  |
| 0.01 | 2.042 |  |
| 0.02 | 2.082 |  |
| 0.03 |  | 2.121 |
| 0.04 |  | 2.158 |
| 0.05 |  | 2.193 |
|  | slope $=4.33$ |  |


|  | $4 \times 4$ sites |  |
| :---: | :---: | :---: |
| $\epsilon^{2}$ |  | $\mathrm{~L} \times$ gap |
| 0 |  | $2.51 \pm 0.02$ |
| 0.01 |  | $2.86 \pm 0.05$ |
| 0.02 |  | $3.109 \pm 0.05$ |
| 0.03 |  | $3.316 \pm 0.05$ |
|  |  |  |


| $6 \times 6$ sites |  |  |  |
| :---: | :---: | :---: | :---: |
|  |  |  |  |
| $\epsilon^{2}$ |  | $\mathrm{~L} \times$ gap |  |
| 0 |  | 2.58 | $\pm 0.03$ |
| 0.01 |  | 3.74 | $\pm 0.17$ |
| 0.02 |  | 4.34 | $\pm 0.06$ |
| 0.03 |  | 4.79 | $\pm 0.13$ |

## Figure Captions

Figure $1 F_{L}$ vs. $\epsilon^{2}$ in one dimension. $\bullet$, $\circ$ and $\Delta$ refer to 4,6 and 8 sites respectively.

Figure $2 F_{L}$ vs. $\epsilon^{2}$ in two dimensions. $\bullet, \circ$ and $\Delta$ refer to $2 \times 2,4 \times 4$ and $6 \times 6$ sites respectively.


Fig. 1


Fig. 2


[^0]:    * This work was supported by the Department of Energy under Contract Number DE-AC0376 SF00515.

