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GROUND STATE ENERGY OF THE ONE-DIMENSIONAL ANISOTROPIC SPIN-1/2 HEISENBERG ANTIFEROMAGNET

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Abstract

The stationary perturbation method yields the ground –state energy of the one-dimensional spin-1/2 anisotropic Heisenberg antiferromagnet. The ground state energy per spin $\left(\frac{E}{N}\right)$ ***as a function of the anisotropic parameter*** (λ) ***for even spins*** (N) $N \geq 6$ ***is found to be*** $-0.25(1+\lambda^2)J$ ***for*** $\lambda = 0.9$. ***This is compareable to Hulthen's solution for the ground state energy per spin*** $(-0.4431479J)$ ***in the thermodynamic limit,*** $N \to \infty$

1.1 INTRODUCTION

The Physics of quantum spin models have attracted a considerable attention over a long period of time [1, 2, 3,5].This interest is due to strong coulomb repulsions between electrons that make up magnetic materials. In the limit of strong coulomb interactions, the electrons are localized and may be well represented by a model Hamiltonian describing a set of interacting spins S_i .The Hamiltonian for such a system is the Heisenberg model:

$$\boldsymbol{H} = \boldsymbol{J}\sum_{\langle i,j\rangle} \boldsymbol{S}_i.\boldsymbol{S}_j \tag{1.1}$$

where the S_i are the spin-S operators, the sum is over nearest neighbour pairs and the dot product $S_i.S_j$ is given by

$$\boldsymbol{S}_i.\boldsymbol{S}_j = \boldsymbol{S}_i^x\boldsymbol{S}_j^x + \boldsymbol{S}_i^y\boldsymbol{S}_j^y + \boldsymbol{S}_i^z\boldsymbol{S}_j^s \tag{1.2}$$

The Heisenberg Hamiltonian (1.1) can be generalized to

$$H = \sum_{\langle i,j\rangle}\left(J_x S_i^x.S_j^x + J_y S_i^y.S_j^y + J_z S_i^z.S_j^z\right) \tag{1.3}$$

This Hamiltonian describes the antiferromagnet (ferromagnetic) Heisenberg model $J \succ 0 (\prec 0)$. It is known as *XYZ* model when $J_x \neq J_y \neq J_z$, the *XY* model when $J_z = 0$ and $J_y = J_z$, and the *XXZ* model when $J_x = J_y$.Using the spin operators $S^{\pm} = S^x \pm iS^y$, the Heisenberg Hamiltonian [Eqn(1.3)] is transformed to

$$H = J\sum_{\langle i,j\rangle}\frac{1}{2}\left(S_i^+S_j^- + S_i^-S_j^+\right) + S_i^ZS_j^Z \tag{1.4}$$

The one dimensional Heisenberg model hasbeen solved exactly using the Bethe Ansatz method [14]. Although the Bethe Ansatz method is limited to one dimension, several methods have been used to study quantum spin models in one and higher dimensions. Among's these methods, numerical and approximation methods have gained recognition over the years [10,11,12]. Using these methods the ground state properties of large finite size lattices can easily be determined.

The aim of this paper is to determine the ground state energy of the one dimensional Heisenberg model for even lattice sites using the stationary perturbation theory. The application of perturbation theory to the physics of correlated electron systems and quantum spin models have been discussed extensively in literature [7, 8,9].Perturbation method relies on us being able to write down convergent or asymptotic series expansion of the observables we are interested in, and therefore works only in restricted ranges of parameter values in the many-body Hamiltonian. The eigenvalues and eigenfunctions can be expanded in a power series in the perturbation parameter λ, that is

$$\boldsymbol{E}_n = \boldsymbol{E}_n^0 + \lambda\boldsymbol{E}_n^1 + \lambda^2\boldsymbol{E}_n^2 + \ldots,$$

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$$|\psi\rangle = |\psi^0\rangle + \lambda|\psi^1\rangle + \lambda^2|\psi^2\rangle + \ldots, \quad (1.5)$$

where in both expressions the first one is the unperturbed one. The remaining section of this paper is organized as follows: in section 1.2,we give a short description of the perturbation method. In sections (1.3-1.6) we compute the ground state energies for even spins and generalize to $N = \infty$ limit, while in section 1.7 the numerical results are presented. In section 1.8 we discuss the results and draw up conclusions.

1.2 Methodology

The Heisenberg Hamiltonian (1.4) in the presence of anisotropic parameter (λ) canbe expressed as

$$H = J\sum_{\langle i,j\rangle}\frac{\lambda}{2}\left(S_i^+S_l^- + S_i^-S_j^+\right) + S_i^ZS_j^Z \quad (1.6)$$

Dividing Eqn (1.6) into two parts, $H = H_o + H_1$,

where $H_o = J\sum_{\langle i,j\rangle} S_i^ZS_j^Z$ (1.7)

and, $H_1 = \frac{-\lambda J}{2}\sum_{\langle i,j\rangle}\left(S_i^\dagger S_j^- + S_i^-S_j^\dagger\right)$ (1.8)

H_o the unperturbed part is the simple Ising model, and its exact ground state is the antiferromagnet Neel State.

H_1 can be treated as a perturbation in λ. $\lambda \in (0,1)$.

The perturbation method involves diagonalizing the matrix[8]

$$\langle\psi^\alpha|H|\psi^\beta\rangle = \langle\psi^\alpha|H_o|\psi^\beta\rangle + \langle\psi^\alpha|H_1|\psi^\beta\rangle + \sum_\delta \frac{\langle\psi^\alpha|H_1|\psi^\beta\rangle\langle\psi^\delta|H_1|\psi^\beta\rangle}{T_o - T_o^\delta} \quad (1.9)$$

The many particle basis $|\psi^\alpha\rangle$ and $|\psi^\beta\rangle$ are eigenstate of H_o and provide the smallest (minimum) energies T_o for a determined number of spins.

The ground state wave function is given by

$$\psi_{gs} = \sum_\alpha C_\alpha\psi^\alpha + \sum_\delta D_\delta\psi^\delta \quad (1.10)$$

In Eqn (1.10) C_α are the zero-order coefficients and are obtained from the diagonalization of the second order Hamiltonian matrix (Eqn(1.9)). Whereas first order coefficients D_δ are given by

$$D_\delta = \sum_\alpha \frac{\langle\psi^\alpha|H_1|\psi^\delta\rangle}{T_o - T_o^\delta}C_\alpha \quad (1.11)$$

Correlation function $\langle S_i^ZS_j^Z\rangle$ and the average magnetic moment can be obtained from the ground state wave function.

$$\langle S_i^ZS_j^Z\rangle = \frac{\langle\psi_{gs}|S_i^Z.S_j^z|\psi_{gs}\rangle}{\langle\psi_{gs}|\psi_{gs}\rangle} \quad (1.12)$$

$$\langle S_i^Z\rangle = \frac{\langle\psi_{gs}|S_i^Z|\psi_{gs}\rangle}{\langle\psi_{gs}|\psi_{gs}\rangle} \quad (1.13)$$

1.3 GROUND STATE ENERGY OF THE 2-SITE HEISENBERG MODEL.

The 2-Site Heisenberg model in the subspace $S^Z = 0$ can be described by the following many-particle states:

$|1\rangle = |1\uparrow,2\downarrow\rangle$, $|2\rangle = |1\downarrow,2\uparrow\rangle$,

$H_o|1\rangle = \frac{-J}{4}$, and $H_o|2\rangle = \frac{-J}{4}|2\rangle$.

That is states $|1\rangle$ and $|2\rangle$ are eigenstate of the unperturbed Hamiltonian H_o, with eigenvalue of $\frac{-J}{4}$. These states are labeled as $|\psi^\alpha\rangle, |\psi^\beta\rangle$ $\alpha, \beta = 1,2$

$$\langle\psi^{\alpha}|H_o|\psi^{\beta}\rangle=\begin{pmatrix}\frac{-J}{4} & 0\\ 0 & \frac{-J}{4}\end{pmatrix} \quad (1.14)$$

Similarly,

$H_1|\psi^1\rangle=\frac{\lambda J}{2}|\psi^2\rangle$, $H_1|\psi^2\rangle=\frac{\lambda J}{2}|\psi^1\rangle$, so that

$$\langle\psi^{\alpha}|H_1|\psi^{\beta}\rangle=\begin{pmatrix}0 & \frac{\lambda J}{2}\\ \frac{\lambda J}{2} & 0\end{pmatrix} \quad (1.15)$$

The second order correction to the ground state is given by

$$\sum_{\delta}\frac{\langle\psi^{\alpha}|H_1|\psi^{\beta}\rangle\langle\psi^{\delta}|H_1|\psi^{\beta}\rangle}{T_o-T_o^{\delta}}=\frac{\langle\psi^{\alpha}|H_1|\psi^{1}\rangle\langle\psi^{1}|H_1|\psi^{\beta}\rangle}{T_o-T_o^{1}}+\frac{\langle\psi^{\alpha}|H_1|\psi^{2}\rangle\langle\psi^{2}|H_1|\psi^{\beta}\rangle}{T_o-T_o^{2}} \quad (1.16)$$

This second order term vanishes because $T_o=T_o^1=T_0^2=\frac{-J}{4}$

$$\langle\psi^{\alpha}|H|\psi^{\beta}\rangle=\begin{pmatrix}\frac{-J}{4} & \frac{\lambda J}{2}\\ \frac{\lambda J}{2} & \frac{-J}{4}\end{pmatrix} \quad (1.17)$$

Let $A=\begin{pmatrix}\frac{-J}{4} & \frac{\lambda J}{2}\\ \frac{\lambda J}{2} & \frac{-J}{4}\end{pmatrix}$

Solving for γ in the equation $Det(A-I\gamma)=0$, gives

$\gamma_1=\frac{-J}{4}+\frac{\lambda J}{2}$, $\gamma_2=\frac{-J}{4}-\frac{\lambda J}{2}$

The ground state energy of the system is

$$E_g=\frac{-J}{4}-\frac{\lambda J}{2} \quad (1.18)$$

For $\lambda=1$ (Isotropic case)

$E_g=\frac{-3J}{4}$ or $-0.75J$.

This result obtained for the isotropic case $(\lambda=1)$ is in good agreement with that obtained using variation wave function approach [11] and Exact calculation [13]

1.4 GROUND STATE ENERGY OF THE 4-SITE HEISENBERG CHAIN

In the subspace $S^z=0$, the 4-site Heisenberg chain has a total number of six basis. If $|\phi\rangle$ is an arbitrary vector in this space, then it of the form

$|\phi\rangle=|1\sigma';2\sigma;3\sigma;4\sigma'\rangle$, where $\sigma,\sigma'=\uparrow,\downarrow$ and are chosen such that the net total spin $S^z=0$.

Eigen states of the unperturbed Hamiltonian H_o which provides the minimum energy T_o for a given number of spins arelabeled as:

$|5\rangle=|1\uparrow,2\downarrow,3\uparrow,4\downarrow\rangle$, $|6\rangle=|1\downarrow,2\uparrow,3\downarrow,4\uparrow\rangle$

That is $H_o|5\rangle=-J|5\rangle$, and $H_o|6\rangle=-J|6\rangle$, where $T_o=T_o^5=T_o^6=-J$

For the remaining four basis states $|i\rangle$, $H_o|i\rangle=0$, $i=1,2,3,4$.

where $T_o^1=T_o^2=T_o^3=T_o^4=0$

Similarly $H|i\rangle=\frac{-\lambda J}{2}(\langle 5|+|6\rangle)$, $i=1,2$ and $H_1|5\rangle=H_1|6\rangle=\frac{-\lambda J}{2}(|1\rangle+|2\rangle+|3\rangle+|4\rangle)$

The ground state energy matrix to a second order in the perturbation parameter λ is found to be

$$\langle\psi^{\alpha}|H|\psi^{\beta}\rangle=\begin{pmatrix}-J-\lambda^2J & -\lambda^2J\\ -\lambda^2J & -J-\lambda^2J\end{pmatrix} \quad (1.19)$$

The ground state energy obtained from Eqn (1.19) is thus

$$E_g = -J - 2\lambda^2 J \tag{1.20}$$

1.5 GROUND STATE ENERGY OF THE 6-SITE HEISENBERG CHAIN

The number of many –particle basis for the six-site Heisenberg chain in the subspace $S_Z = 0$ is given by the relation

$$S = \frac{N!}{\frac{N}{2}!\frac{N}{2}!}$$

For a six-site chain $(N = 6)$, $S = 20$

Of these numbers, many-particle basis of the form $|\psi^i\rangle = |1\sigma, 2\sigma', 3\sigma, 4\sigma', 5\sigma, 6\sigma'\rangle$

with $\sigma = \uparrow, \sigma' = \downarrow$ or $\sigma = \downarrow, \sigma' = \uparrow$ provide the smallest eigenvalue of the unperturbed Hamiltonian H_o .The states are labeled as $|\psi^2\rangle = |1\uparrow, 2\downarrow, 3\uparrow, 4\downarrow, 5\uparrow, 6\downarrow\rangle$, and $|\psi^7\rangle = |1\downarrow, 2\uparrow, 3\downarrow, 4\uparrow, 5\downarrow, 6\uparrow\rangle$ with eigenvalue $\frac{-3J}{2}$

The remaining 18 basis provide eigenvalue of $\frac{-J}{2}$ .That is

$H_o|\psi^i\rangle = \frac{-J}{2}|\psi^i\rangle$, where $\boldsymbol{i = 1,3,4,5,6,8,9,10,\ldots,20}$

By making use of the procedure in sections (1.3) and (1.4), the ground state energy matrix becomes

$$\langle\psi^\alpha|H|\psi^\beta\rangle = \begin{pmatrix} \frac{-3}{2}J - \frac{3}{2}\lambda^2 J & 0 \\ 0 & \frac{-3}{2}J - \frac{3}{2}\lambda^2 J \end{pmatrix} \tag{1.21}$$

The eigenvalues are the diagonal elements of the energy matrix Eqn (1.20). That is

$$E_g = \frac{-3}{2}J - \frac{3}{2}\lambda^2 J \tag{1.22}$$

1.6 GROUND STATE ENERGY OF THE N-SITE HEISENBERG CHAINS (N≥6)

The procedure used in the previous sections can be generalized to include Heisenberg chains of size $N = 8,10,12,14,\ldots$

For $N = 8$

$$\langle\psi^\alpha|H|\psi^\beta\rangle = \begin{pmatrix} -2J - 2\lambda^2 J & 0 \\ 0 & -2J - 2\lambda^2 J \end{pmatrix} \tag{1.23}$$

For $N = 10$

$$\langle\psi^\alpha|H|\psi^\beta\rangle = \begin{pmatrix} -\frac{5}{2}J - \frac{5}{2}\lambda^2 J & 0 \\ 0 & -\frac{5}{2}J - \frac{5}{2}\lambda^2 J \end{pmatrix} \tag{1.24}$$

Thus the ground state energy matrix for the 1D Heisenberg Hamiltonian for antiferromagnetic ordering, in the subspace $S^Z = 0$ is found to be

$$\langle\psi^\alpha|H|\psi^\beta\rangle = \begin{pmatrix} -\frac{N}{4}J(1+\lambda^2) & 0 \\ 0 & -\frac{N}{4}J(1+\lambda^2) \end{pmatrix} \tag{1.25}$$

Where N the number of site is even, $N \geq 6$.

The ground state energy is thus

$$E(\lambda) = \frac{-NJ}{4}(1+\lambda^2) \tag{1.26}$$

1.7 NUMERICAL RESULTS

TABLE 1. Ground state energy per site $(E_n)_P$ obtained using perturbation method. λ is the anisotropic parameter. Values obtained using the same method [12]is shown in the third column for comparison.

λ	$(E_n)_p$	$(E_n)_Q$
0.1	-0.2525	-0.2525
0.2	-0.2600	-0.2600
0.3	-0.2725	-02725
0.4	-0.2900	-0.2900
0.5	-0.3125	-0.3125
0.6	-0.3400	-0.3400
0.7	-0.3725	-0.3725
0.8	-0.4100	-0.4100
0.9	-0.4525	-0.4525

TABLE II. Ground state energy per site $(E_N)_P$ obtained using perturbation method at $J=1$and $\lambda=0.9$. N is the number of sites. Values obtained by Gagliano et al. $(E_N)_L$ [9] and by Bonner and Fisher $(E_N)_D$ [2] using the modified Lanczos and Exact diagonalization method respectively are shown in the third and fourth column for comparison.

N	$(E_n)_p$	$(E_n)_L$	$(E_N)_D$
6	-2.7150	-2.8027	-2.8028
8	-3.6200	-3.6511	-3.6511
10	-4.5250	-4.5154	-4.5155
12	-5.4300	-5.3874	-5.3874
14	-6.3550	-6.2635	-6.2040
16	-7.2400	-7.1423	-7.0903
18	-8.1450	-8.0227	-7.9766
20	-9.0500	-8.9044	-8.8629
22	-9.9550	-9.7869	-9.7492
24	-10.8600	-10.6355	-10.6355

TABLE III. Comparison between ground state energy per site (E/N)obtained using perturbation method and other approximate and numerical methods in the limit $N\to\infty$

Reference	Method	**E/N**
[13]	RSRG	-0.44378
[9]	Modified Lanczos	$-0..4431\pm0.001$
[1]	Exact diagonalization	$-0..4431\pm0.003$
[14]	Bethe Ansatz	$-0..4431475$
[12]	Variational monte carlo	$-0..423729$
Present work	Perturbation method	$-0..45250$

1.8 DISCUSSION

The ground state energies of the one dimensional spin-1/2 Heisenberg model in the In the subspace $S_Z=0$ have been computed using the stationary perturbation theory. The ground state energy of $-0.75J$ obtained for a two spin system is the same with that obtained by Oles[11]using the variational wave function approach.

In section 1.4, the ground state energy of $-1.98J$ for $\lambda=0.7$,compare nicely with the values of $-2.00J$ obtained by Gagliano et al.[9], Bonner and Fisher[2] and Ehika et al.[13].In Table 1numerical results for the ground state energy per site is presented for different values of the anisotropic parameter (λ).The values shown in the second column using perturbation method, compare nicely with the values obtained by a Parkinson and Farnell [12] as shown in the third column. The ground state energy matrix Eqn.(1.25) is of second order and is a diagonal matrix. In table II, we display results for the ground state

energies for $N \geq 6$ up to $N = 24$ sites. Our results is shown in the second column and is in good agreement with values obtained by Gaglianio et al.[9], Bonner and Fisher[2]as shown in the third and fourth column respectively.
In table III, the ground state energies per site (E/N) for the limit $N \to \infty$ obtained using various approximation and numerical methods are shown. Our result of $-0.45250J$ compare favourably with these other methods.

1.9 CONCLUSION

We have computed the ground state energies for the one-dimensional Heisenberg model using the stationary perturbation theory. The ground state energy matrix obtained in our study is of second order in the anisotropic parameter (λ), and is a diagonal matrix. Our result of $-J-2\lambda^2 J$ at $\lambda = 1$ for the four-site Heisenberg antiferromagnetic reproduces the result of $-3J$ for the four-site Heisenberg chain obtained by Kung et al.[10], using the projector Monte Carlo method.

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