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ODD NUMBER OF COUPLED ANTIFERROMAGNETIC ANISOTROPIC HEISENBERG CHAINS: SPIN WAVE THEORY[1]

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ABSTRACT

The effect of the chain and perpendicular anisotropies on the energy gap for odd number of coupled quantum spin-1/2 antiferromagnetic anisotropic Heisenberg chains is investigated using a spin wave theory. The energy gap opens above a critical anisotropic value. The known results of the isotropic case have been obtained.

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The discovery of materials such as $(VO)_2P_2O_7$ [1] and $Sr_2Cu_4O_6$ [2] which contain weakly coupled arrays of metal-oxide-metal ladders, has stimulated interest in coupled-chain Heisenberg, Hubbard, and t-J systems.

From the theoretical point of view, it has been suggested that systems with an even number of isotropic chains are gapped spin liquids, while odd number of isotropic chains are gapless [3]. This idea was supported by limited exact diagonalization results for three chains [4], mean field results for two and four chains [5], and a density matrix renormalization group (DMRG) results for odd and even number of isotropic chains [6]. To our knowledge the anisotropic case has not been studied up to now.

The purpose, of this letter, is to investigate the odd number of coupled quantum spin-1/2 antiferromagnetic anisotropic Heisenberg chains, using a spin wave theory [7].

The antiferromagnetic anisotropic Heisenberg model on the system (Fig.1) is denoted as follows

$$H = J_{//}^{xy} \sum_{\langle i,j\rangle_{//}} \left(S_i^x S_j^x + S_i^y S_j^y + \alpha_{//} S_i^z S_j^z\right) + J_{\perp}^{xy} \sum_{\langle i,j\rangle_{\perp}} \left(S_i^x S_j^x + S_i^y S_j^y + \alpha_{\perp} S_i^z S_j^z\right) \qquad (1)$$

where the sums run over first nearest neighbours $<i,j>_{//}$ along the chains and $<i,j>_{\perp}$ perpendicular to the chains. $J_{//}^{xy}$ and $J_{\perp}^{xy}$ are the positive antiferromagnetic exchange constants. $\alpha_{//} = J_{//}^{z} / J_{//}^{xy}$ and $\alpha_{\perp} = J_{\perp}^{z} / J_{\perp}^{xy}$ are the chain and perpendicular anisotropy parameters respectively.

The antiferromagnetic spin wave theory by Anderson and Kubo [7] is applied to the Hamiltonian (1). Thus, we divide a lattice with NM sites (N is the sites number of the chain, and M is the anisotropic chains number) into two sublattices (A) and (B) such that each site of (A) is adjacent only to sites of (B). Then S_l and S_m denote the spin operators of the sublattices (A) and (B) respectively. The Holstein-Primakoff transformation is applied to these operators. This transformation is defined by

$$\begin{cases} S_l^z = S - a_l^+ a_l \\ S_l^- = \sqrt{2S}\, a_l^+ \sqrt{1 - \dfrac{a_l^+ a_l}{2S}} \end{cases} \qquad \begin{cases} S_m^z = -S + b_m^+ b_m \\ S_m^- = \sqrt{2S} \sqrt{1 - \dfrac{b_m^+ b_m}{2S}}\, b_m \end{cases} \qquad (2)$$

where a_l, a_l^+, b_m and b_m^+ are the creation and annihilation operators of spin deviations for sublattices (A) and (B) respectively and satisfy the Bose commutation relations, namely

$$[a_l, a_{l'}^+] = \delta_{l,l'}$$
$$[b_m, b_{m'}^+] = \delta_{m,m'} \qquad (3)$$
$$[a_l, b_m^+] = [a_l^+, b_m] = [a_l, b_m] = [a_l^+, b_m^+] = 0$$

We substitute Eq.(2) into Eq.(1) and the part of only lowest order terms denotes H^{swt}. Then

$$H^{swt} = S \sum_{\substack{i=1,N \\ j=1,2,3}} \left\{ (a_{i,j} b_{i+1,j} + a_{i,j}^+ b_{i+1,j}^+) + \alpha_{//} (a_{i,j}^+ a_{i,j} + b_{i+1,j}^+ b_{i+1,j}) \right\}$$
$$+ \alpha^{xy} S \sum_{i=1,N} \left\{ (a_{i,1} b_{i,2} + a_{i,1}^+ b_{i,2}^+ + a_{i,3} b_{i,2} + a_{i,3}^+ b_{i,2}^+) + \alpha_\perp (a_{i,1}^+ a_{i,1} + a_{i,3}^+ a_{i,3} + 2 b_{i,2}^+ b_{i,2}) \right\} \qquad (4)$$
$$- 3NS^2 \alpha_{//} - 2NS^2 \alpha^{xy} \alpha_\perp$$

where α^{xy} $(= J_\perp^{xy} / J_{//}^{xy})$ is the anisotropy parameter.

We apply the Fourier transformation

$$a_l = \sqrt{\frac{2}{MN}} \sum_k e^{-ikl} a_k$$
$$b_m = \sqrt{\frac{2}{MN}} \sum_k e^{ikm} b_k \qquad (5)$$

where k is a vector in a reciprocal lattice of a sublattice. Using Eq.(5) the commutation relations become

$$[a_k, a_{k'}^+] = [b_k, b_{k'}^+] = \delta_{k,k'}$$
$$[a_k, b_{k'}] = [a_k^+, b_{k'}] = [a_k, b_{k'}^+] = [a_k^+, b_{k'}^+] = 0 \qquad (6)$$

Then the Eq.(4) is given by

$$H^{swt} = 2S \sum_k \left\{ (\alpha_{//} + \frac{2}{3} \alpha^{xy} \alpha_\perp)(a_k^+ a_k + b_k^+ b_k) + (\cos k_x + \frac{2}{3} \alpha^{xy} \cos k_y)(a_k^+ b_k^+ + a_k b_k) \right\} \qquad (7)$$
$$- 3NS^2 (\alpha_{//} + \frac{2}{3} \alpha^{xy} \alpha_\perp)$$

Therefore, the Eq.(7) can be generalized to an arbitrary odd number of coupled anisotropic chains. So, we get

$$H^{swt} = 2S \sum_k \left\{ (\alpha_{//} + \frac{M-1}{M} \alpha^{xy} \alpha_\perp)(a_k^+ a_k + b_k^+ b_k) + (\cos k_x + \frac{M-1}{M} \alpha^{xy} \cos k_y)(a_k^+ b_k^+ + a_k b_k) \right\} \qquad (8)$$
$$- MNS^2 (\alpha_{//} + \frac{M-1}{M} \alpha^{xy} \alpha_\perp)$$

This Hamiltonian can be diagonalized by the Bogoliubov transformation

$$U = \mathrm{Exp}[-\sum_k \theta_k (a_k^+ b_k^+ - a_k b_k)]$$
$$\alpha_k = U a_k U^+ = a_k \cosh(\theta_k) + b_k^+ \sinh(\theta_k) \qquad (9)$$
$$\beta_k^+ = U b_k^+ U^+ = a_k \sinh(\theta_k) + b_k^+ \cosh(\theta_k)$$

As Eq.(9) is an unitary transformation, the commutation relations (6) are preserved, namely

$$[\alpha_k, \alpha_{k'}^+] = [\beta_k, \beta_{k'}^+] = \delta_{k,k'}$$
$$[\alpha_k, \beta_{k'}] = [\alpha_k^+, \beta_{k'}] = [\alpha_k, \beta_{k'}^+] = [\alpha_k^+, \beta_{k'}^+] = 0 \tag{10}$$

Then the Hamiltonian (8) becomes

$$H^{swt} = \sum_k \left\{ -2S(\alpha_{//} + \frac{M-1}{M}\alpha^{xy}\alpha_\perp) + W^{swt}(k)(\alpha_k^+\alpha_k + \beta_k^+\beta_k) + W^{swt}(k) \right\}$$
$$- MNS^2(\alpha_{//} + \frac{M-1}{M}\alpha^{xy}\alpha_\perp) \tag{11}$$

where the dispersion relation is given by

$$W^{swt}(k) = 2S((\alpha_{//} + \frac{M-1}{M}\alpha^{xy}\alpha_\perp)^2 - (\cos k_x + \frac{M-1}{M}\alpha^{xy}\cos k_y)^2)^{\frac{1}{2}}. \tag{12}$$

Therefore $\alpha_k, \alpha_k^+, \beta_k$ and β_k^+ are the creation and annihilation operators of the elementary excitation, and the ground state is their vacuum state. Then the spin deviation averaged in the ground state, denotes by Δs, has the form

$$\Delta S = \langle a_l^+ a_l \rangle = \frac{1}{2}\int_{-\pi}^{\pi} \frac{dk_x}{2\pi} \left\{ \frac{1}{M} \sum_{\substack{k_y = -\pi + j\frac{2\pi}{M} \\ (j=1,M)}} \frac{2S(\alpha_{//} + \frac{M-1}{M}\alpha^{xy}\alpha_\perp)}{W^{swt}(k_x, k_y)} \right\} - \frac{1}{2}. \tag{13}$$

The ground state energy per spin is

$$\frac{E_{gs}^{swt}}{MN} = -(\alpha_{//} + \frac{M-1}{M}\alpha^{xy}\alpha_\perp)S(S+1) + \frac{1}{2}\int_{-\pi}^{\pi} \frac{dk_x}{2\pi} \left\{ \frac{1}{M} \sum_{\substack{k_y = -\pi + j\frac{2\pi}{M} \\ (j=1,M)}} W^{swt}(k_x, k_y) \right\}. \tag{14}$$

Moreover, the energy gap has the form

$$E_g = W^{swt}(k_x = 0, k_y = 0) = 2S[(\alpha_{//} + \frac{M-1}{M}\alpha^{xy}\alpha_\perp)^2 - (1 + \frac{M-1}{M}\alpha^{xy})^2]^{\frac{1}{2}}. \tag{15}$$

From Fig.2, the spin wave theory results for the quantum spin-1/2 antiferromagnetic anisotropic Heisenberg chain are in a good qualitative agreement with the known results given by Parkinson et al.[8]. Indeed, the energy gap has a linear behaviour for $\alpha_{//} >> 1$, while near $(\alpha_{//})_c = 1$, it has a simple power law form

$$E_g(\alpha_{//}) \approx c(\alpha_{//} - 1)^g \tag{16}$$

where $c = \sqrt{2}$ is the constant and the exponent g=1/2.

The spin deviation, which is displayed in Fig.3, shows that the three coupled chains system is disordered for any value of the α^{xy} at a fixed value of the chain and perpendicular anisotropies, $\alpha_{//} = \alpha_{\perp} = 1$. While for M>3, the systems exhibit two finite critical anisotropies values $\alpha_{c_1}^{xy}$ and $\alpha_{c_2}^{xy}$; for $\alpha_{c_1}^{xy} < \alpha < \alpha_{c_2}^{xy}$ the system is ordered, but elsewhere, it is disordered. Furthermore, for infinite M, we get the case of a square lattice which presents a finite anisotropic value $\alpha_c^{xy} = 0.033$ below which the square lattice is disordered, while it is ordered for $\alpha^{xy} > \alpha_c^{xy}$. These results are in excellent agreement with those of Sakai et al.[9]. In addition, a relevant result is also obtained; the spin deviation diverges for single chain, while it is finite for any finite odd number of chains.

The ground state energy given in eq.(14), decreases with increasing chains number, or increasing value of the anisotropy α^{xy}. For $\alpha^{xy} = 0$, we recover the usual spin-wave energy per spin for the isotropic chain ($E_g^{swt} = -0.4317$) rather close to the exact result ($E_g = -0.4432$)[10]. At the point $\alpha^{xy} = 1$, for infinite M, we get ($E_g^{swt} = -0.658$) which is in a qualitative agreement with Monte Carlo calculations ($E_g = -0.669$)[11].

The effect of the $\alpha_{//}$ and $\alpha_{\perp}$ anisotropies on the energy gap is given in Fig.4. There exists a critical anisotopic value ($\alpha_c^{xy} = \frac{1-\alpha_{//}}{\alpha_{\perp}-1}\frac{M}{M-1}$) for each anisotropy value $\alpha_{\perp} > 1$ at a

fixed value $\alpha_{//} \leq 1$, from which the energy gap opens. The energy gap has a linear behaviour for $\alpha^{xy} >> \alpha_c^{xy}$, while near α_c^{xy}, it has a simple power law form, namely

$$E_g(\alpha^{xy}) = C_1(\alpha^{xy} - \alpha_c^{xy})^{g_1} \tag{17}$$

where the constant is given by $C_1 \approx [\frac{\alpha_\perp - 1}{\alpha_\perp}(\alpha_{//} + 1 + \alpha_c^{xy}\frac{M-1}{M}(\alpha_\perp + 1))]^{\frac{1}{2}}$ and the exponent $g_1 = 1/2$. Then the critical anisotropic value α_c^{xy} decreases with increasing perpendicular anisotropy $\alpha_\perp$. For $\alpha_{//} = \alpha_\perp = 1$, the energy gap vanishes. This result is in excellent agreement with density matrix renormalization group (DMRG) results [6]. Equivalent results are obtained for any odd number of anisotropic chains. However, the anisotropic chains number favours the energy gap opening much more at a fixed value of the $\alpha_{//}$ and $\alpha_\perp$ anisotropy parameters.

In conclusion, using spin wave theory, we have studied the energy gap for odd number of anisotropic chains. The energy gap opens for $\alpha^{xy} > \alpha_c^{xy}$. The known results of the isotropic case have been obtained.

Acknowledgments

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Figure captions

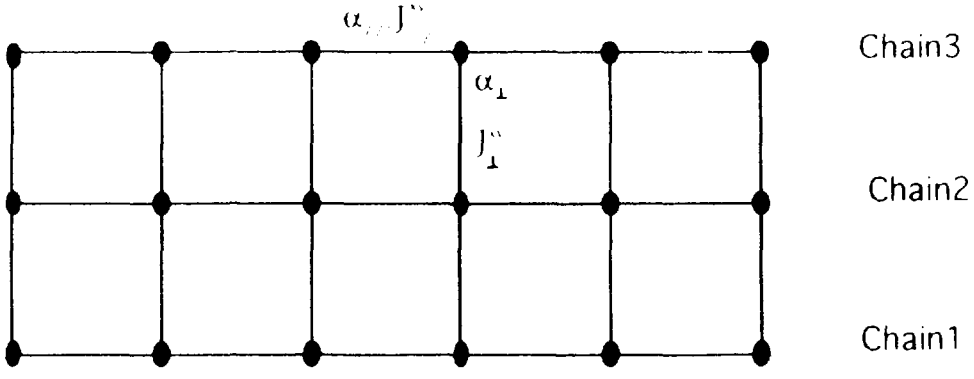
Fig.1: The antiferromagnetic anisotropic system (three coupled spin chains).

Fig.2: The dependence of the energy gap Eg on the chain anisotropy $\alpha_{//}$.

Fig.3: The dependence of the spin deviation ΔS at a fixed values of the chain and perpendicular anisotropies ($\alpha_{//} = \alpha_{\perp} = 1$). The number accompanying each curve denotes the number of coupled chains.

Fig.4: The dependence of energy gap Eg on the anisotropy α^{xy} at a fixed value of the chain anisotropy ($\alpha_{//} = 0.5$). The number accompanying each curve denotes the value of the perpendicular anisotropy $\alpha_{\perp}$

Fig.1


$\alpha_{\parallel} J''_{\parallel}$
$\alpha_{\perp}$
$J''_{\perp}$
Chain3
Chain2
Chain1

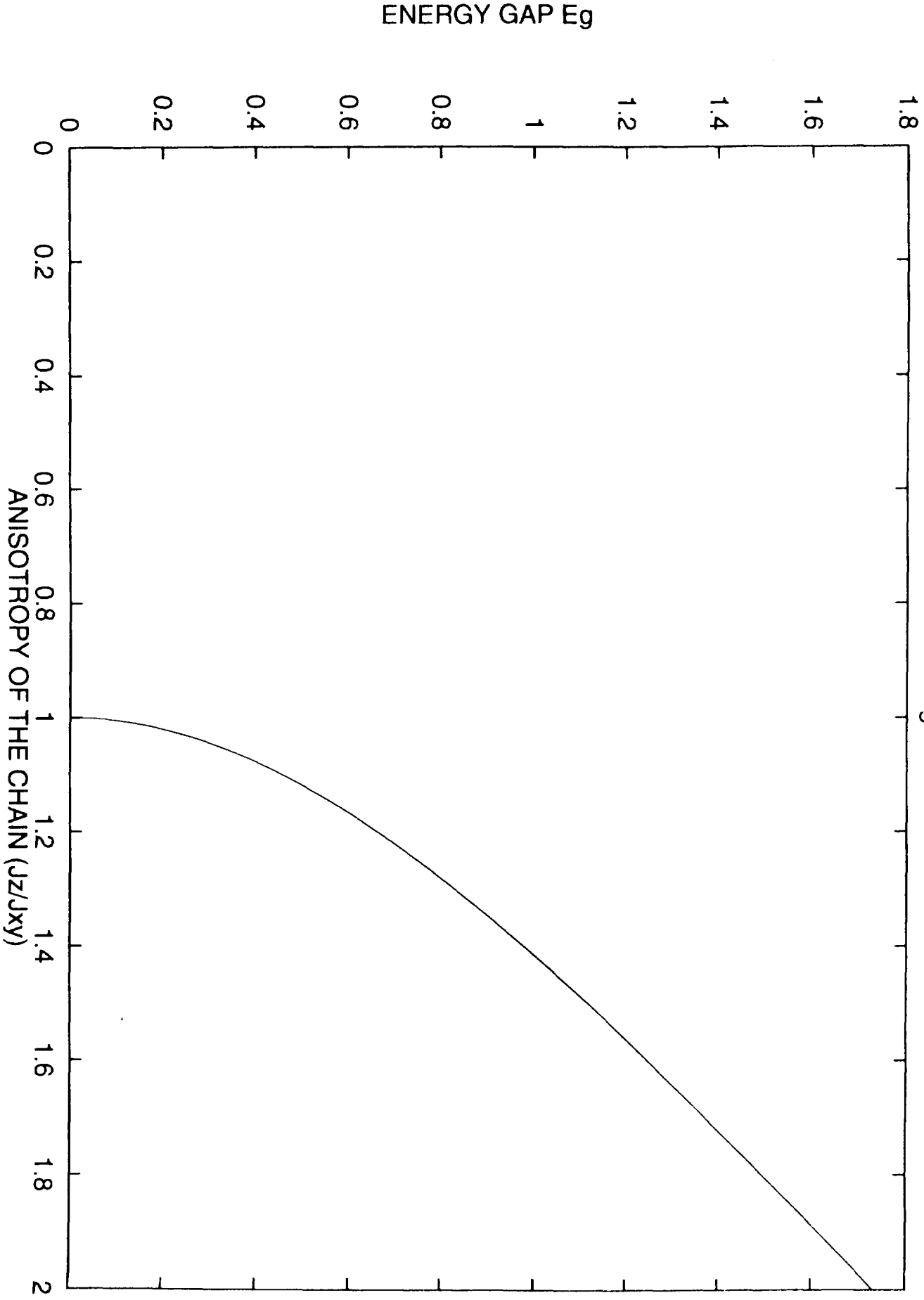

ENERGY GAP Eg
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
ANISOTROPY OF THE CHAIN (Jz/Jxy)
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2

Fig.2

Fig.3

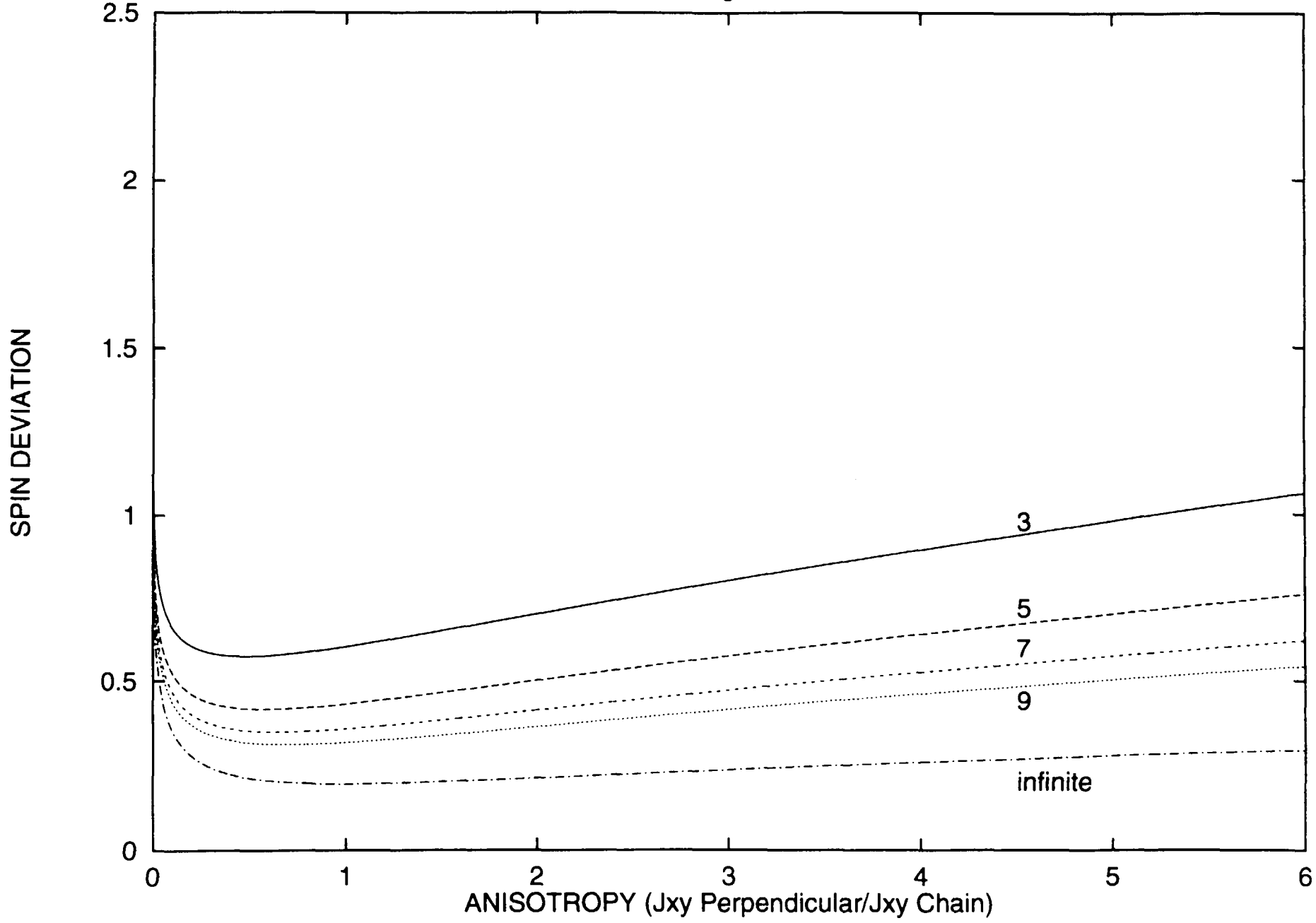
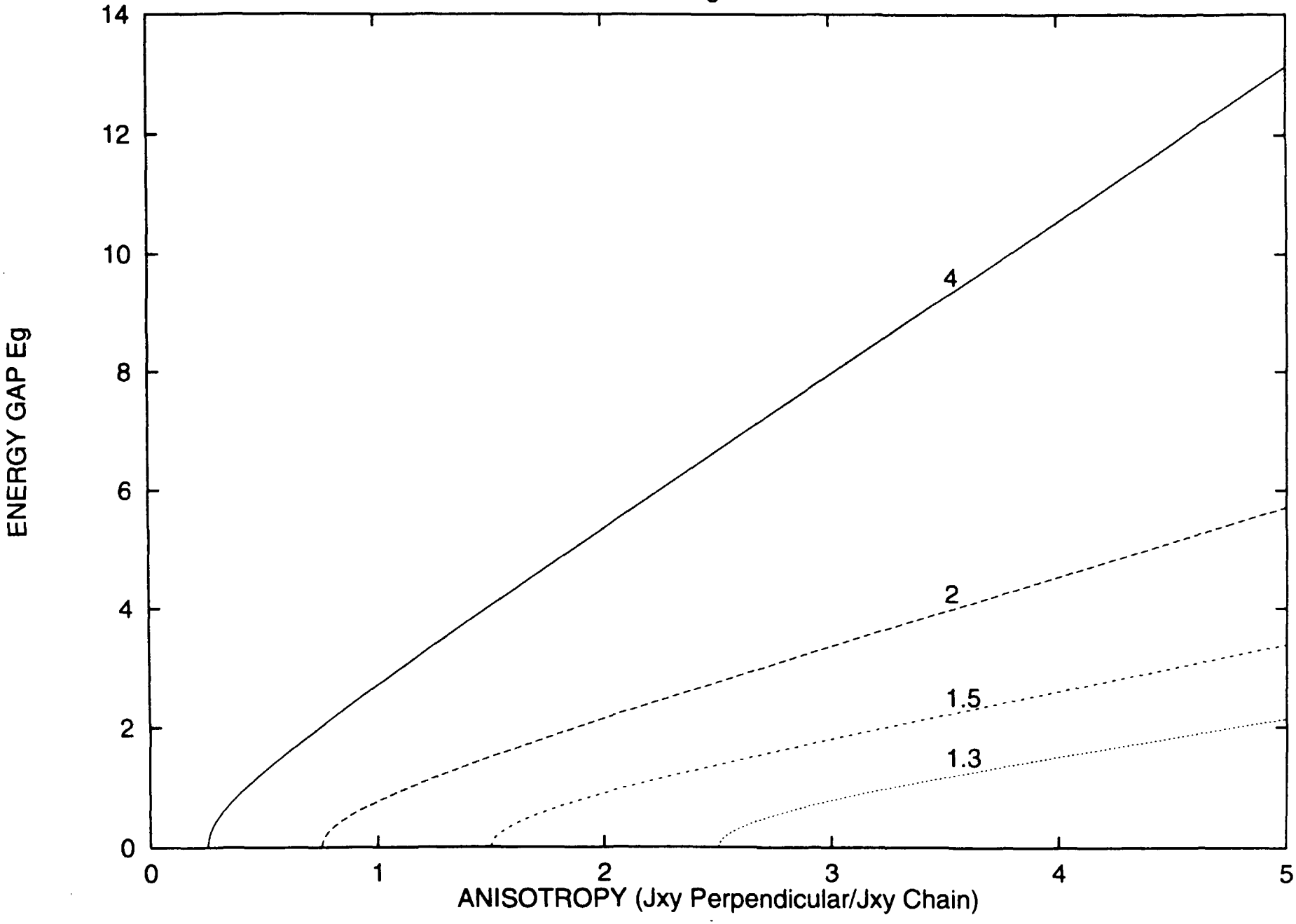

2.5
2
1.5
1
0.5
0
0
1
2
3
4
5
6
SPIN DEVIATION
ANISOTROPY (Jxy Perpendicular/Jxy Chain)
3
5
7
9
infinite

Fig.4


14
12
10
8
6
4
2
0
0
1
2
3
4
5
ENERGY GAP Eg
ANISOTROPY (Jxy Perpendicular/Jxy Chain)
4
2
1.5
1.3