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# INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS



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MIRAMARE-TRIESTE

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INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

# A MEAN FIELD STUDY OF THE QUASI-ONE-DIMENSIONAL ANTIFERROMAGNETIC ANISOTROPIC HEISENBERG MODEL[1]

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## ABSTRACT

The effect of the chain and the dimer anisotropies on the ground state energy and the energy gap of the spin-1/2 quasi-one-dimensional antiferromagnetic Heisenberg model is investigated using a mean field theory. The dependence of the magnetization and the effective hopping parameters on the anisotropy $\alpha^{xy}(= J_{\perp}^{xy}/J_{//}^{xy})$ are presented for several values of the chain anisotropy. However, such a system exhibits a transition from antiferromagnetic ordered to disordered phases for arbitrary chain anisotropy and dimer anisotropy.

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# 1- Introduction

The antiferromagnetic anisotropic Heisenberg ladders (two coupled spin chains) are relevant to the understanding of how the physics evolves from the purely one-dimensional systems to two-dimensional. Also, the quantum spin S=1/2 antiferromagnetic anisotropic Heisenberg model on the ladder can model the magnetic properties of systems such as the vanadyl pyrophosphate[1], $(VO)_2P_2O_7$.

From the theoretical point of view, two main reasons are behind the increasing interest in the antiferromagnetic anisotropic Heisenberg ladder. The Haldane conjecture[2,3] that the energy gap of the elementary excitations of chains depends on whether the spin is integer or half-integer. It is well known[4] that the spin one-half 1D Heisenberg model is gapless. This prediction has been supported by many theoretical studies, which are, for example, finite-size scaling[5], numerical diagonalizations[6,7], Monte Carlo calculations[8], analysis of an exactly solvable model[9], a variational method[10], the numerical real-space quantum renormalization groups[11], etc. However, it is not clear how the gap behaves when a transverse coupling, $J_\perp(J_\perp^z, J_\perp^{xy})$ is turned on between the two chains of the antiferromagnetic anisotropic Heisenberg ladder. The second reason is the discovery of high critical temperature superconductors (HTcS)[12]. The interest for these systems is due to belief that the 2D Heisenberg model describes the antiferromagnetic interactions in the undoped copper-oxygen planes of HTcS.

The problem of a plane of coupled spin-1/2 chains was studied by several authors[13-17]. For the ladder, no broken symmetry is expected to occur because of the 1D nature of the system. Indeed, the finite size in the transverse direction will bring different physics than the two-dimensional Heisenberg model. We believe that the gap starts to be non-zero for any finite $\alpha^{xy}(\alpha^{xy} = J_\perp^{xy} / J_{//}^{xy})$ due to the finite size in the transverse direction[18]. In the limit of large $\alpha^{xy}$ the system is equivalent to weakly coupled singlets and the energy gap is given in leading order by the singlet-triplet energy separation. The first term of the energy gap is linear in $\alpha^{xy}$.

Our aim is to investigate, the quantum spin-1/2 antiferromagnetic anisotropic Heisenberg chains, ladders, and arbitrary odd and even number of coupled antiferromagnetic anisotropic Heisenberg chains problems using a mean field approach.

# 2-Model and Method

## a-Model

The antiferromagnetic anisotropic Heisenberg model on the ladder is denoted as follows

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

where the sums run over first nearest neighbours $\langle i,j\rangle_{//}$ along the chains and $\langle i,j\rangle_{\perp}$ 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 anisotropy parameters of the chains and dimers, respectively. In the following the periodic boundary conditions are imposed.

## b-Method

The two-dimensional generalization of Wigner-Jordan transformation[19], can be easily implemented in the case of the antiferromagnetic anisotropic Heisenberg ladder. One gets, following the notation of the Fig.(1)

$$S_{i,1}^{-} = C_{i,1} \mathrm{Exp}\left[ i\pi \sum_{k=0}^{i-1} \left(n_{k,1} + n_{k,2}\right)\right] \quad (2)$$

for the chain 1, and

$$S_{i,2}^{-} = C_{i,2} \mathrm{Exp}\left[ i\pi \left( \sum_{k=0}^{i} n_{k,1} + \sum_{k=0}^{i-1} n_{k,2} \right)\right] \quad (3)$$

for the chain 2. The indices i run along the chains. The Hamiltonian is now written in this fermion representation. One finds the following spinless interacting fermion Hamiltonian

$$\begin{aligned} H = & -\frac{J_{//}^{xy}}{2} \sum_{i,\delta} \left[ C_{i,1} \mathrm{Exp}\left(-i\phi_{i,i+\delta}(1)\right) C_{i+\delta,1}^{+} + C_{i,2} \mathrm{Exp}\left(-i\phi_{i,i+\delta}(2)\right) C_{i+\delta,2}^{+} \right] \\ & -\frac{J_{\perp}^{xy}}{2} \sum_{i} \left( C_{i,1} C_{i,2}^{+} + C_{i,2} C_{i,1}^{+} \right) \\ & + J_{//}^{xy} \alpha_{//} \sum_{i,j=1,2,\delta} \left( n_{i,j} - \frac{1}{2} \right) \left( n_{i+\delta,j} - \frac{1}{2} \right) + J_{\perp}^{xy} \alpha_{\perp} \sum_{i} \left( n_{i,1} - \frac{1}{2} \right) \left( n_{i,2} - \frac{1}{2} \right) \end{aligned} \quad (4)$$

The phases $\phi$ are given as follows

$$\begin{aligned} \phi_{i,i+1}(1) &= \pi n_{i,2} \\ \phi_{i,i-1}(1) &= -\pi n_{i-1,2} \\ \phi_{i,i+1}(2) &= \pi n_{i+1,1} \\ \phi_{i,i-1}(2) &= -\pi n_{i,1} \end{aligned} \quad (5)$$

and $\delta$ refers to the first nearest neighbours of a given site. The flux due to the XY term of the Hamiltonian(4) is taken to be $\pi$ per plaquette on average. For the Ising, one chooses $\langle C_{i,j}C^{+}_{i+\delta,j}\rangle = |\langle C_{i,j}C^{+}_{i+\delta,j}\rangle| E_{xp}[-i\varphi_{i,i+\delta}(j)]$ and $\langle C_{i,j}C^{+}_{i,j+\delta}\rangle = |\langle C_{i,j}C^{+}_{i,j+\delta}\rangle| E_{xp}[-i\varphi_{j,j+\delta}(j)]$ (j=1,2). In the following, we set $\langle C_{i,j}C^{+}_{i+\delta,j}\rangle = Q, \langle C_{i,j}C^{+}_{i,j+\delta}\rangle = P$, and the staggered magnetization $m = 2 < n_{i,j} > -1$. The sum over $\varphi$'s around one plaquette is also taken to be $\pi$ on average. The bipartite character and the different phases on each link of the system are summarized in Fig.(2), and using the equality $Exp(i\pi n_{i,j}) = 1 - 2n_{i,j}$, the mean field Hamiltonian is written as follows

$$
\begin{aligned}
H = {} & \frac{J^{xy}_{//}}{2}\sum_i \left(C^{+}_{i,1}Exp[-i\pi]C_{i+1,1} + C^{+}_{i,1}C_{i-1,1} + C^{+}_{i,2}C_{i+1,2} + C^{+}_{i,2}Exp[i\pi]C_{i-1,2}\right) \\
& + \frac{J^{xy}_{\perp}}{2}\sum_i \left(C^{+}_{i,1}C_{i,2} + C^{+}_{i,2}C_{i,1}\right) + \frac{J^{xy}_{//}}{2}\alpha_{//}\sum_{i,j=1,2,\delta}\left(m n_{i,j} - m n_{i+\delta,j} + \frac{m^2}{2}\right) \\
& + \frac{J^{xy}_{\perp}}{2}\alpha_{\perp}\sum_i \left(m n_{i,1} - m n_{i,2} + \frac{m^2}{2}\right) \\
& + J^{xy}_{//}\alpha_{//}\sum_i \left(QC^{+}_{i,1}Exp[-i\pi]C_{i+1,1} + QC^{+}_{i,1}C_{i-1,1} + QC^{+}_{i,2}C_{i+1,2} + QC^{+}_{i,2}Exp[i\pi]C_{i-1,2} + Q^2\right) \\
& + J^{xy}_{\perp}\alpha_{\perp}\sum_i \left(PC^{+}_{i,1}C_{i,2} + PC^{+}_{i,2}C_{i,1} + P^2\right)
\end{aligned}
\tag{6}
$$

where a bipartite lattice due to antiferromagnetic correlations is used, in Fig.(2). We get

$$H = \sum_k E_{\pm}(k)\alpha^{+}_{k,\pm}\alpha_{k,\pm} \tag{7}$$

in k-space where the fermionic operator $\alpha_k$ is obtained from $C_k$ through the diagonalization of the Hamiltonian(6).The dispersion relation is given by

$$E_{\pm}(k) = \pm\left[m^2(J^{xy}_{//}\alpha_{//} + \frac{J^{xy}_{\perp}}{2}\alpha_{\perp})^2 + J^{xy}_{//}{}^2\left(1+2Q\alpha_{//}\right)^2 Sin^2 k_x + (\frac{J^{xy}_{\perp}}{2})^2\left(1+2P\alpha_{\perp}\right)^2 Cos^2 k_y\right]^{1/2}. \tag{8}$$

Thus the ground state energy has the form

$$E_{GS} = J^{xy}_{//}\alpha_{//}Q^2 + \frac{J^{xy}_{\perp}}{2}\alpha_{\perp}P^2 + \frac{m^2}{4}\left(J^{xy}_{//}\alpha_{//} + \frac{J^{xy}_{\perp}}{2}\alpha_{\perp}\right) - \frac{1}{2}\int\frac{dk_x}{2\pi}\left[\frac{1}{2}\sum_{k_{y=0,\pi}} E_{+}(k)\right] \tag{9}$$

where $J^{xy}_{\perp}$ is divided by a factor 2 since the periodic boundary conditions used in the transverse direction count $J^{xy}_{\perp}$ twice. The minimization of the ground state energy with respect to m, Q and P gives the following three self-consitent equations

$$m = \int \frac{dk_x}{2\pi} [\frac{1}{2} \sum_{k_y=0,\pi} \frac{m(J_{//}^{xy}\alpha_{//} + \frac{J_{\perp}^{xy}}{2}\alpha_{\perp})}{E_+(k)}]$$

$$Q = \frac{1}{2}\int \frac{dk_x}{2\pi} [\frac{1}{2} \sum_{k_y=0,\pi} \frac{J_{//}^{xy}(1+2Q\alpha_{//})Sin^2 k_x}{E_+(k)}] \qquad (10)$$

$$P = \frac{1}{2}\int \frac{dk_x}{2\pi} [\frac{1}{2} \sum_{k_y=0,\pi} \frac{\frac{J_{\perp}^{xy}}{2}(1+2P\alpha_{\perp})Cos^2 k_y}{E_+(k)}]$$

The integration is over the first Brillouin zone. Furthermore, the energy gap is given by

$$E_g(\alpha^{xy}) = E_+((k_x,k_y)=(0,\pi)) = J_{//}^{xy}[m^2(\alpha_{//} + \frac{\alpha_{\perp}}{2}\alpha^{xy})^2 + (\frac{\alpha^{xy}}{2})^2(1+2P\alpha_{\perp})^2]^{\frac{1}{2}} \qquad (11)$$

where $\alpha^{xy}$(=Jxy Dimer/Jxy Chain) is the anisotropy parameter.

# 3-Results and Discussion

We find that the antiferromagnetic anisotropic Heisenberg chain is ordered for any value of the chain anisotropy, $\alpha_{//}$. At low anisotropy $\alpha_{//} \leq 0.3$, the energy gap is very weak (for example for $\alpha_{//} = 0.19$, Eg=0.001) Fig.(8.b). However, the finite critical anisotropic value $(\alpha_{//})_c$ below which the energy gap vanishes, does not exist. For this reason we choose the zero magnetization, due to the spin wave theory results[20,21] which goes beyond the mean field approach. Within this solution (m=0) the energy gap is zero for $\alpha_{//} \leq 1$. However, for $\alpha_{//} > 1$, the result of the mean field theory is in qualitative agreement with the numerical diagonalization results[6].

For the ladder our results are presented in two important cases as follows:

## a-Weak chain anisotropy : $\alpha \leq 1$

The numerical solutions of the equations (10) are the flux-phase[22], with zero magnetization and the Néel-flux-phase with finite magnetization. For nonzero magnetization, the quantum fluctuations due to spin wave excitations would have drastic repercussions on the value of the magnetization. As in one dimensional, these fluctuations destroy long-range order. Indeed, for the ladder, the corrections to the magnetization in the standard spin wave theory can be calculated and are found to be logarithmically singular

$$\Delta\langle S^z\rangle \approx \int \frac{dk}{k} \approx -\infty \qquad (12)$$

This implies that spin wave theory is not self-consistent and no long-range order can occur at zero temperature. So the flux-phase solution (m=0) is more adequate to describe the antiferromagnetic correlations even if its ground state energy is slightly higher than that of the Néel-flux-phase state as shown in Fig.(5). The parameters Q and P which are displayed in Fig.(4) show no simple dependence on $\alpha^{xy}$. The energy gap, which is displayed in Fig.(3), has a linear behaviour in $\alpha^{xy} >> 1$. This is in a good qualitative agreement with the simple limit $\alpha^{xy} = \infty$ . For sufficiently small $\alpha^{xy}$ , $E_g(\alpha^{xy})$ has a simple power law form namely

$$Eg(\alpha^{xy}) \approx c(\alpha^{xy})^g \qquad (13)$$

where the constant C=0.76 and the exponent g=1 for different values of the chain and dimer anisotropies. From Fig.(3), it is clear that the antiferromagnetic coupling $J_\perp^z$ opens much more the energy gap than does the antiferromagnetic coupling $J_\perp^{xy}$. Therefore, our results obtained for $\alpha_{//} = 1$, are in a good agreement with the Lanczos techniques and Monte Carlo results[14], and the density matrix renormalization group results[13,16].

## b- Strong chain anisotropy : $\alpha > 1$

In this case, the Néel-flux-phase state has a nonzero magnetization for $\alpha^{xy} \langle \alpha_c^{xy}$. The different parameters of this state are displayed in Fig.(7). The energy gap is found to go to a finite limit when $\alpha^{xy} \to 0$. The finite magnetization in this state implies broken rotational symmetry. The Néel-flux-phase states give the same dispersion for $\alpha^{xy} \rangle \alpha_c^{xy}$. Thus, we observe in Fig.(6) that the antiferromagnetic coupling $J_\perp^z$ favours the antiferromagnetic order much more than does the antiferromagnetic coupling $J_\perp^{xy}$, and the system exhibits a transition from antiferromagnetic ordered to disordered phases for arbitrary chain and dimer anisotropies.

In addition, the effect of the size is important on the energy gap opening. Fig.(8) shows that the energy gap of the quasi-one-dimensional spin system is much more open than the spin chain system one.

Special cases are displayed in Figs.(9,10). Indeed we show that, for Ising dimer and anisotropic chains ( $J_\perp^z \neq 0$ and $J_\perp^{xy} = 0$), the ladder is ordered for any value of $\alpha_{//}$. However

for XY dimer model and anisotropic chains ( $J_{\perp}^{z} = 0$ and $J_{\perp}^{xy} \neq 0$), the ladder is disordered for $\alpha_{//} < (\alpha_{//})_c$, while it is ordered for $\alpha_{//} > (\alpha_{//})_c$. In both cases there exists a nonzero energy gap, but the Ising dimer model is dominant for $\alpha_{//} > (\alpha_{//})^c$, while XY dimer model is dominant for $\alpha_{//} < (\alpha_{//})^c$.

Moreover, we have also applied the mean field approach to an arbitrary odd and even number of the coupled quantum spin-1/2 antiferromagnetic anisotropic Heisenberg chains. We find from the anisotropy-gap dependence presented in Figs.(11a,11b), that for even number of chains, the results are in a good agreement with the density matrix renormalization group results[16] and the mapping procedure results[17]. While, for odd number of chains, the results are in disagreement with the known results[16,17]. Indeed, in both cases even and odd, and for zero magnetization and finite magnetization the energy gap increases with increasing the chains number. From these pictures the surprising result is that the two dimensional spatially anisotropic Heisenberg model open a gap for arbitrary anisotropy (also for the isotropic case). So, in the flux-phase (m=0), this is in disagreement with the known results[18]. While, in the Néel-flux-phase $m \neq 0$, the dependence of the energy gap on the $\alpha^{xy}$ is still controversial.

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# Figure Captions

**Fig.1.**The antiferromagnetic anisotropic ladder system.

**Fig.2.**The flux per plaquette is equal to $\pi$ on average.

**Fig.3.**The dependence of the energy gap Eg on the anisotropy $\alpha^{xy}$ at a fixed value of the chain anisotropy $\alpha_{//} = 0.8$. The number accompanying each curve denotes the value of dimer anisotropy $\alpha_{\perp}$.

**Fig.4.**The dependence of the effective hopping parameters Q, P on the $\alpha^{xy}$ at $\alpha_{//} = 0.8$ and $\alpha_{\perp} = 1$.

**Fig.5.**The dependence of the ground state energies Eg on the $\alpha^{xy}$ at $\alpha_{//} = 0.8$ and $\alpha_{\perp} = 1$. (a) correspond to the solution m=0, while (b) correspond to the solution m>0.

**Fig.6.**The dependence of the energy gap Eg and magnetization m on the anisotropy $\alpha^{xy}$ at $\alpha_{//} = 1.5$. The number accompanying each curve denotes the value of the dimer anisotropy $\alpha_{\perp}$ .

**Fig.7.**The dependence of the energy gap Eg, magnetization m, and effective hopping parameters Q, P on the $\alpha^{xy}$ at $\alpha_{//} = 1.5$ and $\alpha_{\perp} = 1$.

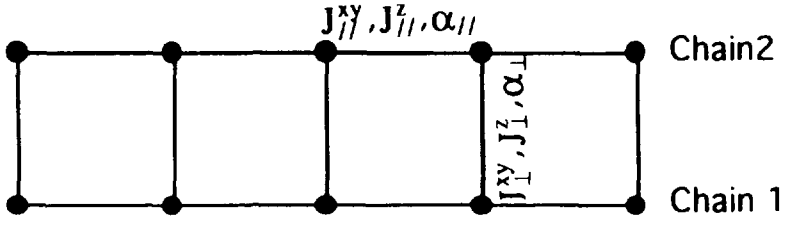
**Fig.8.**The dependence of the energy gap Eg on the chain anisotropy $\alpha_{//}$. (a) correspond to two chains coupled at $\alpha^{xy} = 1$ the number accompanying each curve denotes the value of the dimer anisotropy $\alpha_{\perp}$, while (b) correspond to the antiferromagnetic anisotropic Heisenberg chain.

**Fig.9.**The dependence of the energy gap Eg on the chain anisotropy $\alpha_{//}$ at $\alpha^{xy} = 1$ (a) correspond to $J_{\perp}^{z} \neq 0$ and $J_{\perp}^{xy} = 0$, while (b) correspond to $J_{\perp}^{z} = 0$ and $J_{\perp}^{xy} \neq 0$.

**Fig.10.**The dependence of the magnetization on the chain anisotropy $\alpha_{//}$ at (a') correspond to $J_{\perp}^{z} \neq 0$ and $J_{\perp}^{xy} = 0$,while (b') correspond to $J_{\perp}^{z} = 0$ and $J_{\perp}^{xy} \neq 0$.

**Fig.11.**The dependence of the energy gap Eg at fixed values of the chain and dimer anisotropies, $\alpha_{//} = \alpha_{\perp} = 1$, (Fig.11a) correspond to the zero magnetization (m=0), while (Fig.11b) correspond to finite magnetization ( $m \neq 0$). The number accompanying each curve denotes the number of coupled chains.

Fig.1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Chain2
$J^{xy}_{\perp}, J^{z}_{\perp}, \alpha_{\perp}$
Chain 1

Fig.2

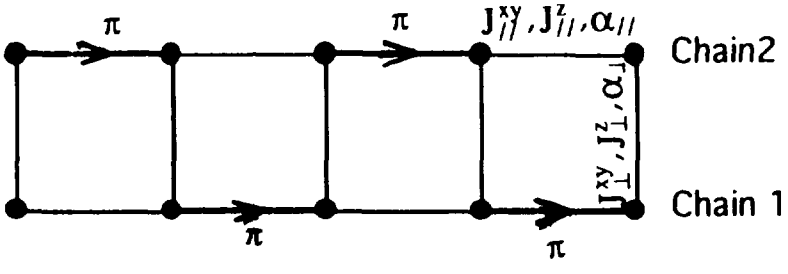
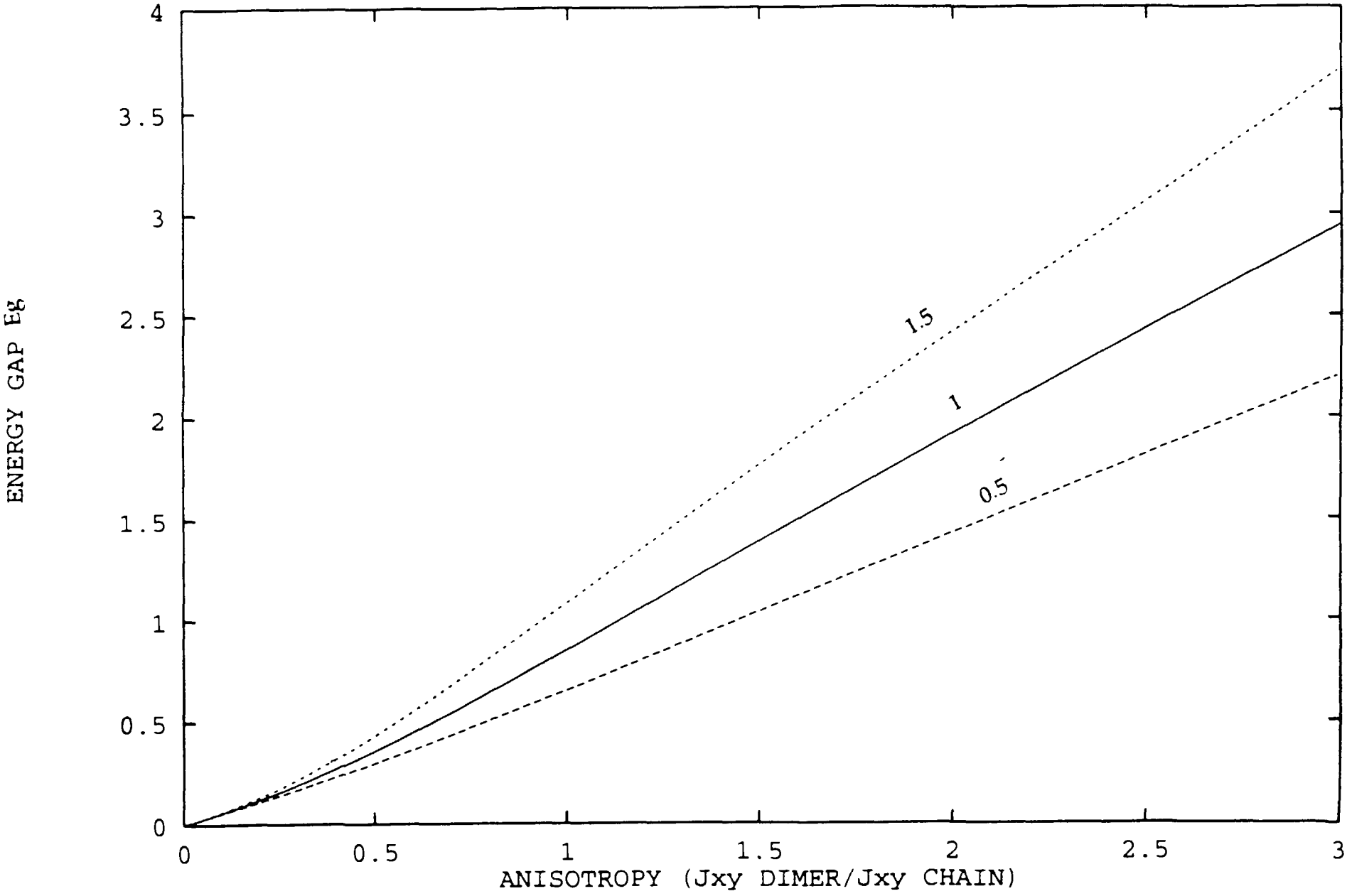

π
π
$J^{xy}_{//}, J^{z}_{//}, \alpha_{//}$
Chain2
$J^{xy}_{\perp}, J^{z}_{\perp}, \alpha_{\perp}$
Chain 1
π
π

Fig. 3


ENERGY GAP Eg
ANISOTROPY (Jxy DIMER/Jxy CHAIN)
1.5
1
0.5
0
0.5
1
1.5
2
2.5
3
3.5
4

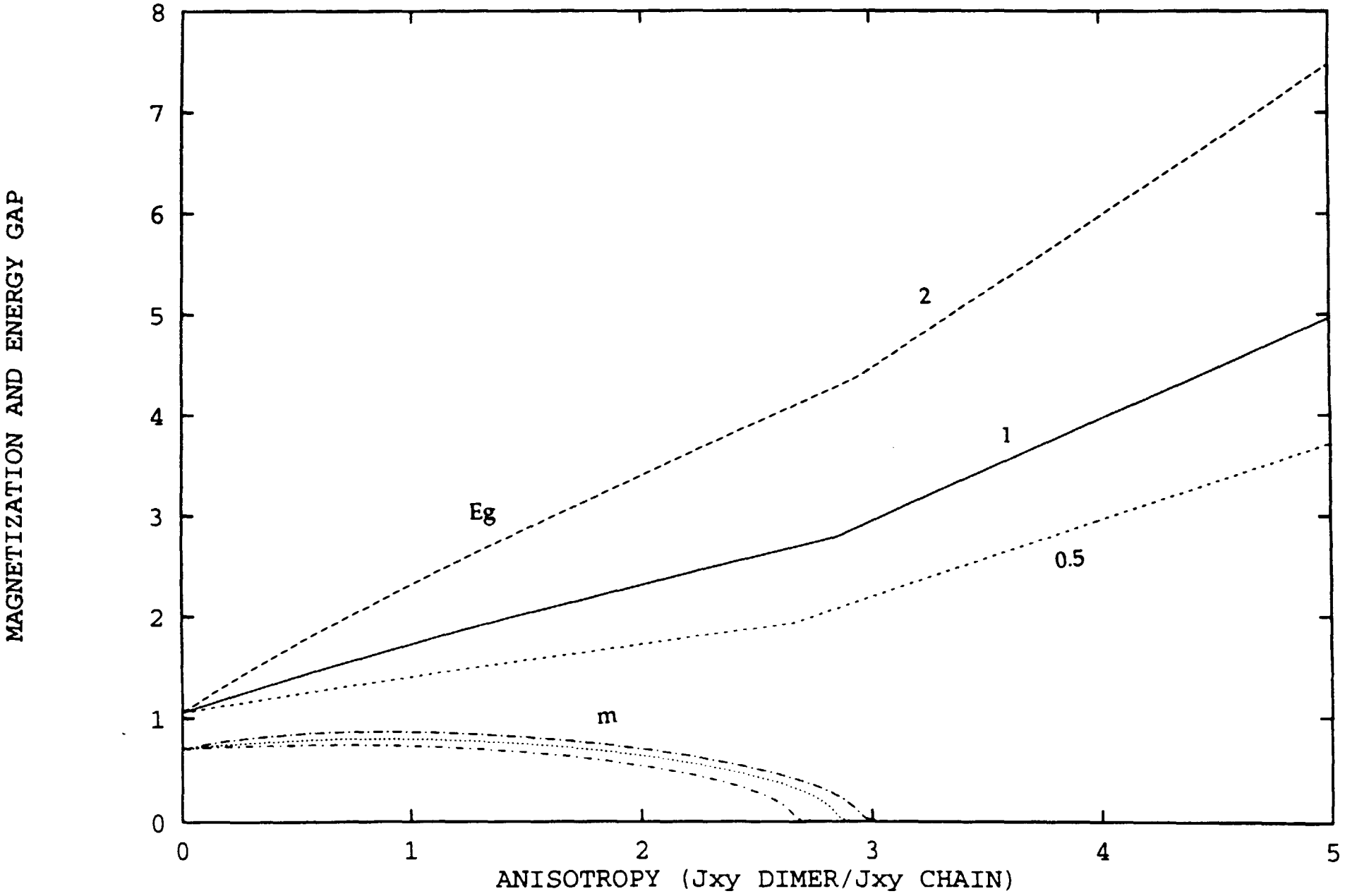
EFFECTIVE HOPPING PARAMETERS
0
0.05
0.1
0.15
0.2
0.25
0.3
0.35
0.4
0.45
0.5
0
0.5
1
1.5
2
2.5
3
ANISOTROPY (JXY DIMER/JXY CHAIN)
P
Q

Fig.4

GROUND STATE ENERGIES Eg
-1.2
-1.1
-1
-0.9
-0.8
-0.7
-0.6
-0.5
-0.4
-0.3
0
0.5
1
1.5
2
2.5
3
ANISOTROPY(Jxy dimer/Jxy chain)
(a)
(b)

Fig. 5

Fig.6


MAGNETIZATION AND ENERGY GAP
ANISOTROPY (Jxy DIMER/Jxy CHAIN)
Eg
m
2
1
0.5
0
1
2
3
4
5
6
7
8

ENERGY GAP Eg ,MAGNETIZATION m ,EFFECTIVE HOPPING PARAMETERS Q,P




Fig.7

Fig.8

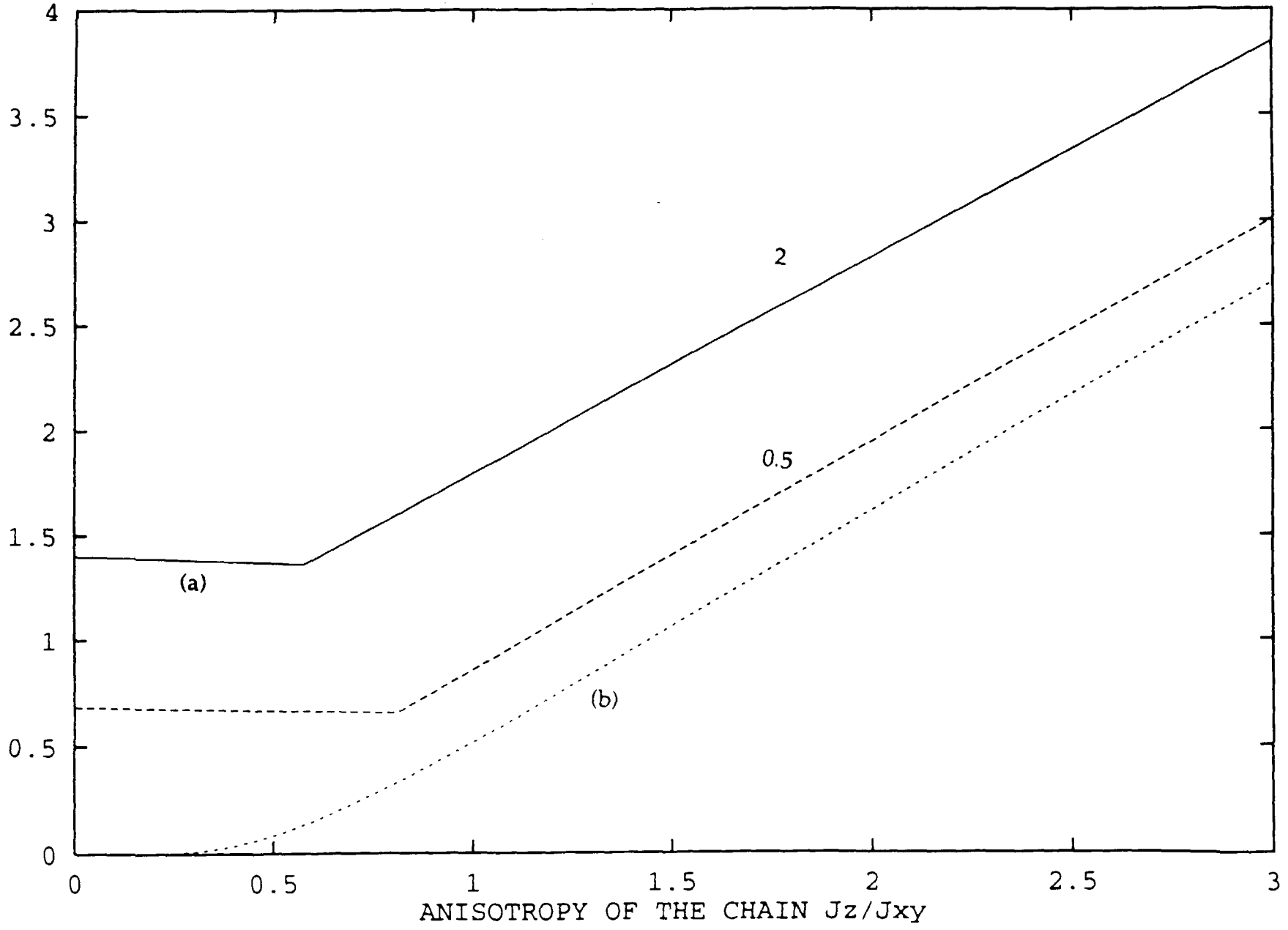
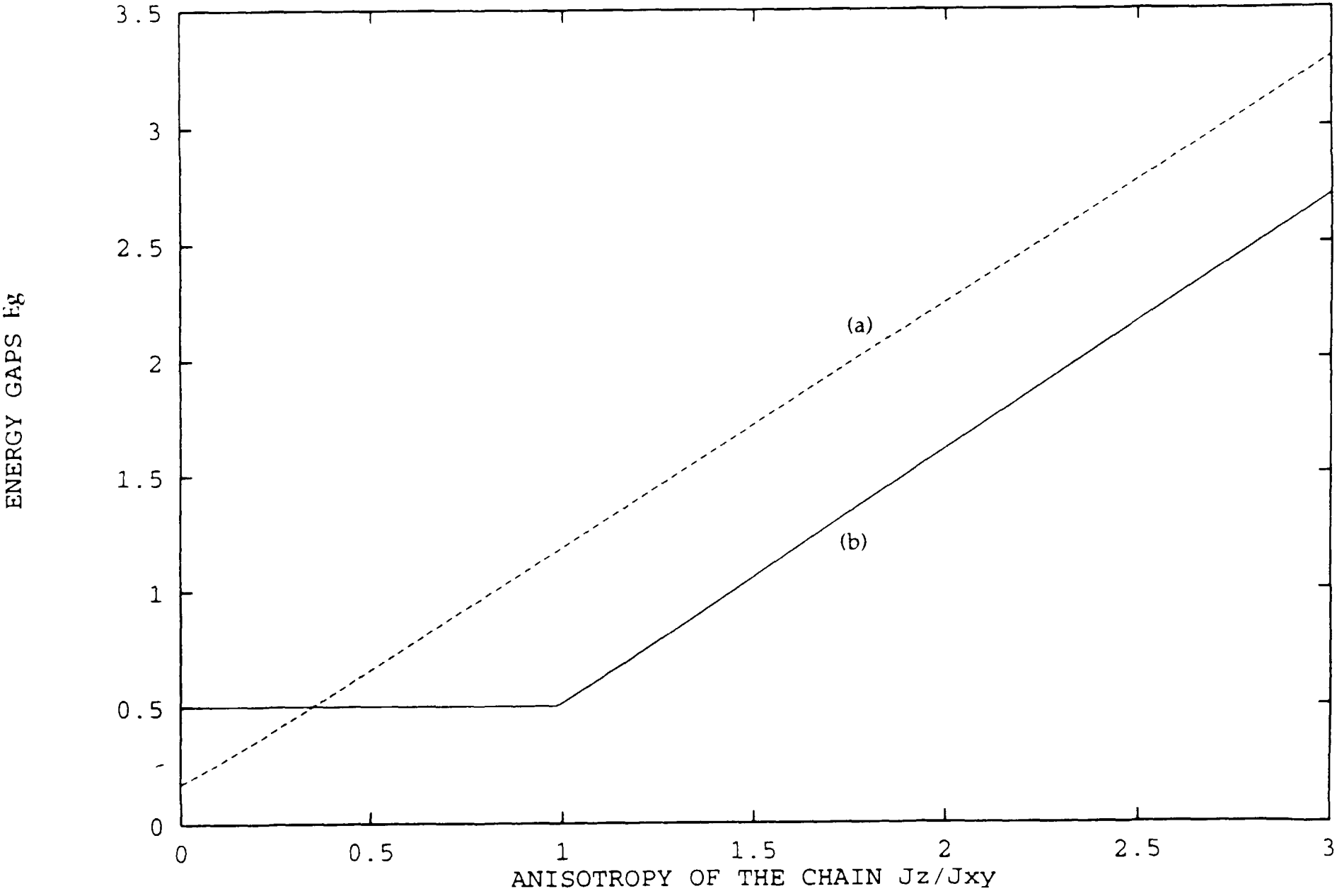

4
3.5
3
2.5
2
1.5
1
0.5
0
0
0.5
1
1.5
2
2.5
3
ENERGY GAP Eg
ANISOTROPY OF THE CHAIN Jz/Jxy
2
0.5
(a)
(b)

Fig.9


ENERGY GAPS Eg
3.5
3
2.5
2
1.5
1
0.5
0
0
0.5
1
1.5
2
2.5
3
ANISOTROPY OF THE CHAIN Jz/Jxy
(a)
(b)

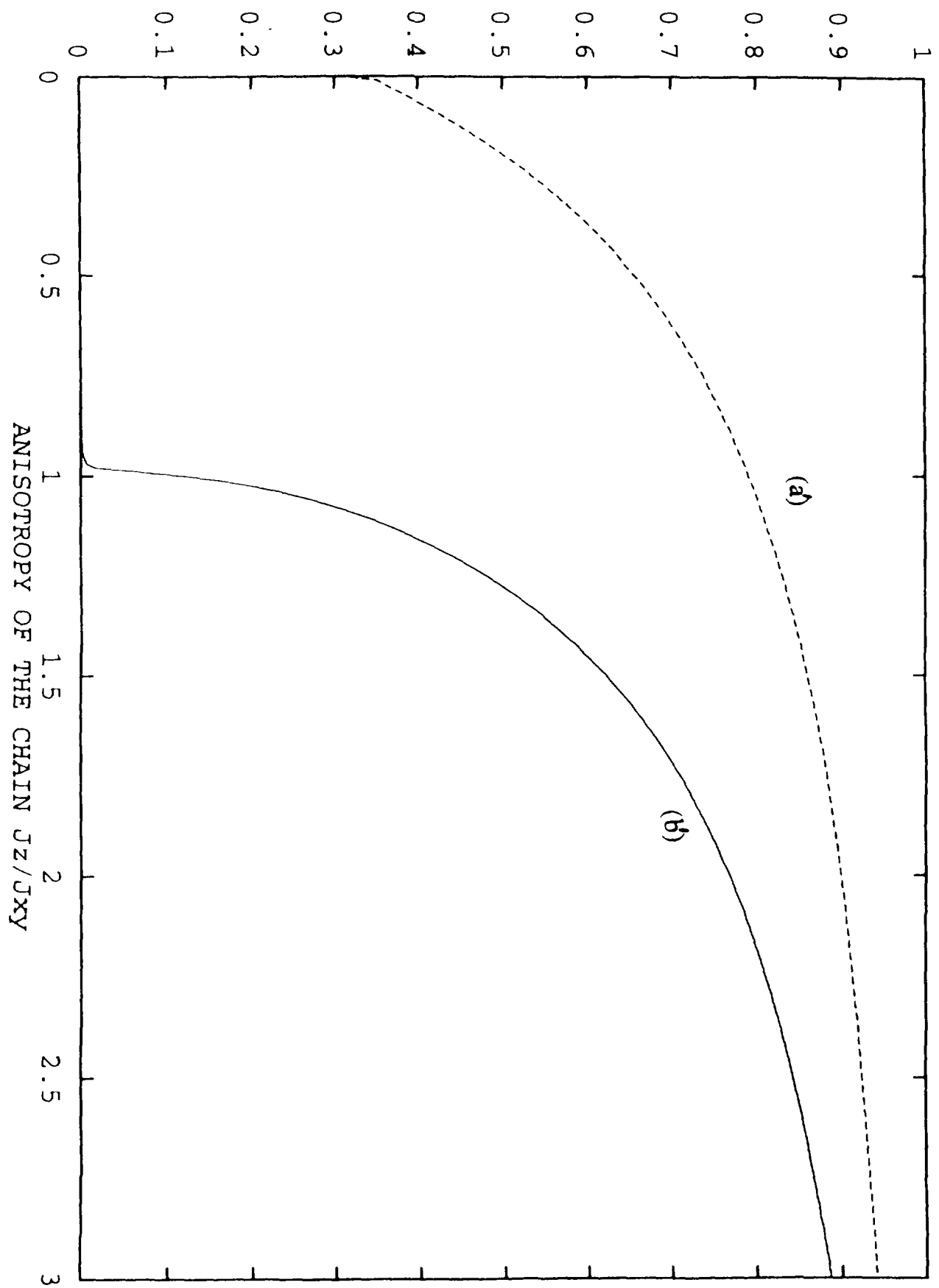
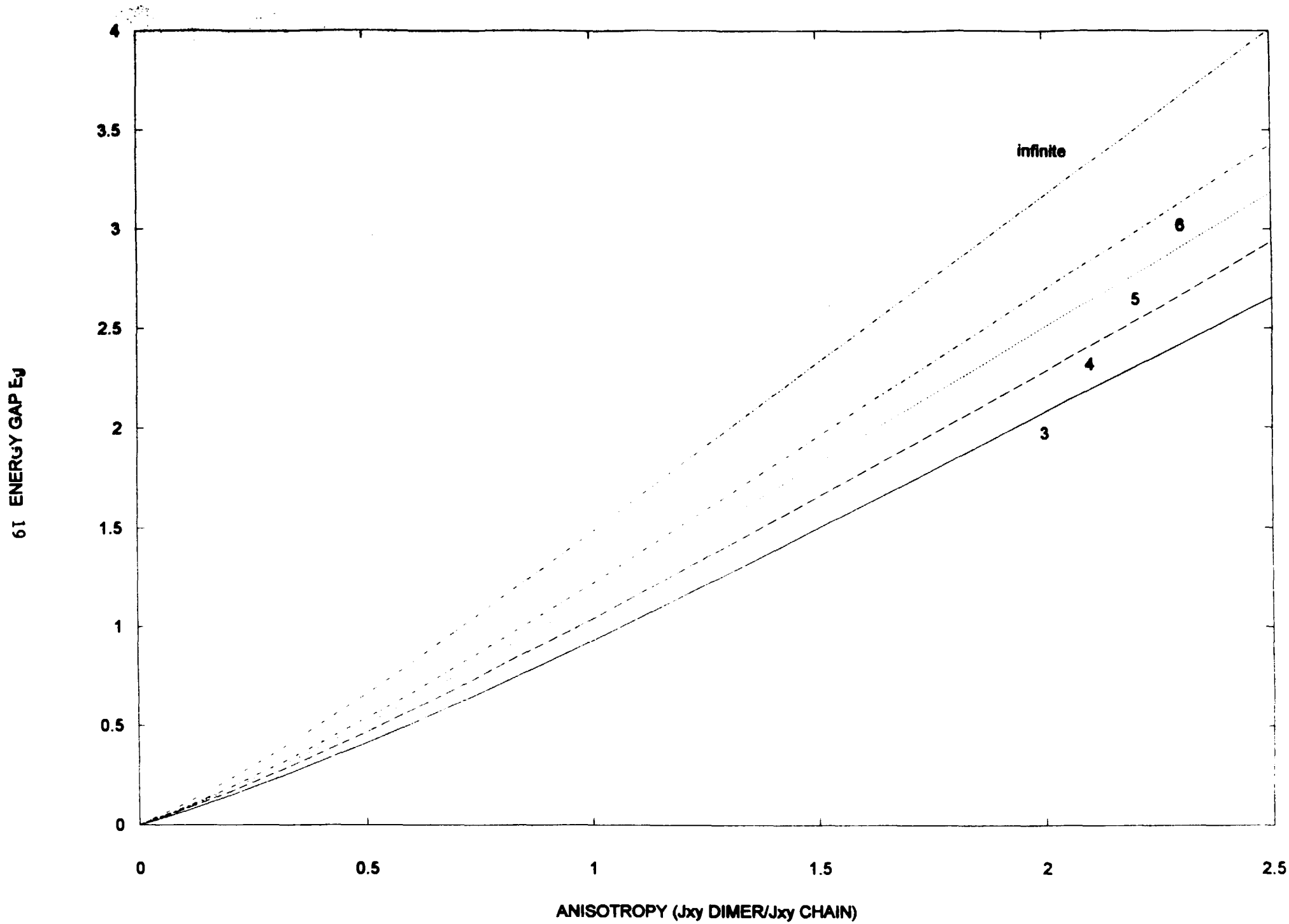
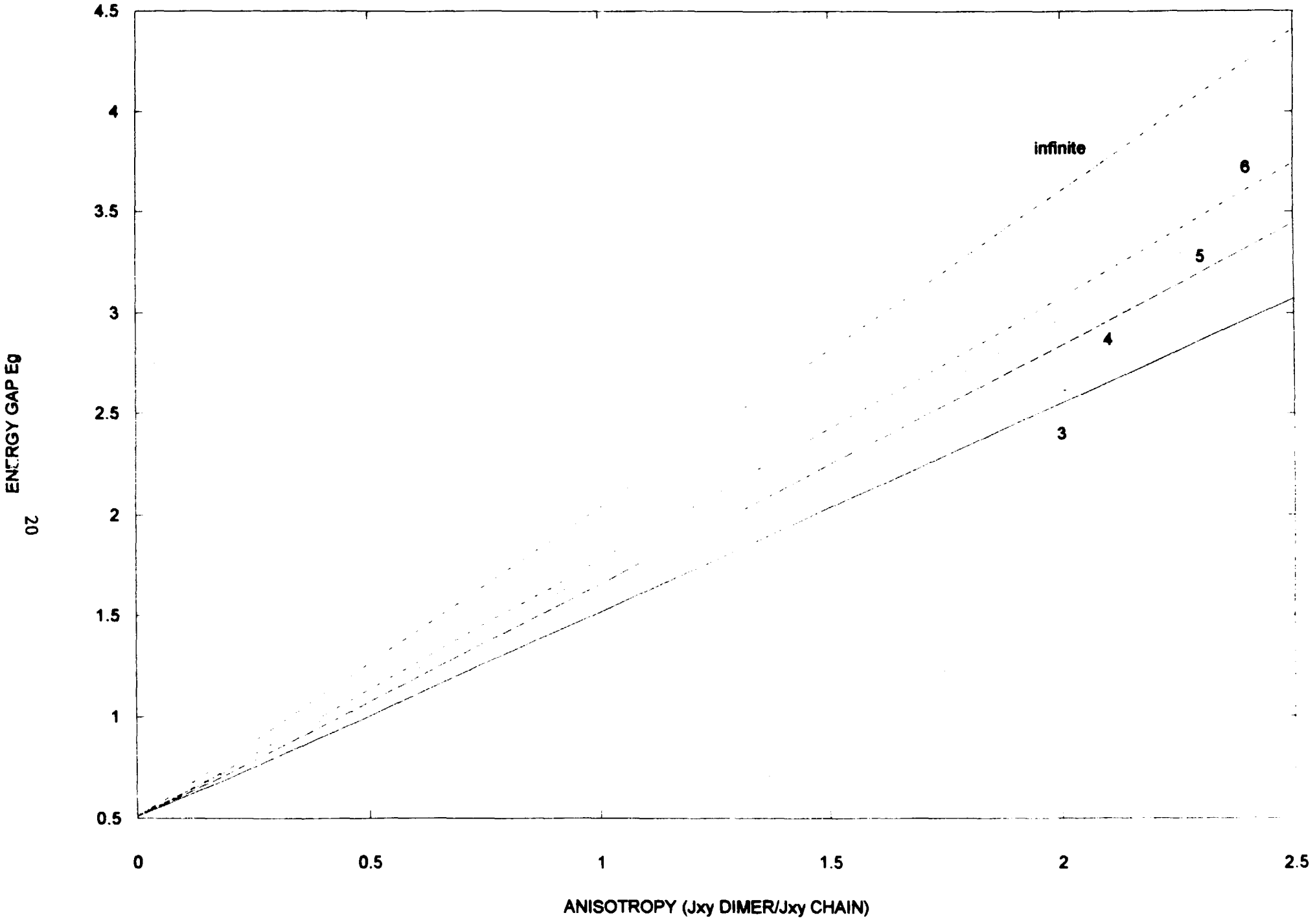

LOCAL MAGNETIZATIONS m
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0
0.5
1
1.5
2
2.5
3
ANISOTROPY OF THE CHAIN Jz/Jxy
(a)
(b)

Fig.10

Fig.11a


4
3.5
3
2.5
2
1.5
1
0.5
0
0
0.5
1
1.5
2
2.5
infinite
6
5
4
3
ENERGY GAP Ej
ANISOTROPY (Jxy DIMER/Jxy CHAIN)


4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
0.5
1
1.5
2
2.5
ENERGY GAP Eg
ANISOTROPY (Jxy DIMER/Jxy CHAIN)
infinite
6
5
4
3