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Spin-correlation functions of the anisotropic XY chain

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We have calculated the spin-correlation functions (in the x, y, and z directions) in the linear spin-$\frac{1}{2}$ XY system for both isotropic and anisotropic couplings. The study of zero-temperature correlation functions shows that a long-range order develops in the direction in which the coupling is stronger, but no such ordering exists for isotropic systems. We have studied the temperature variation of inverse correlation lengths in these directions and it has been found that at $T=0$ all the correlation lengths (ξ_x, ξ_y, ξ_z) diverge in the isotropic case. On the other hand, in the anisotropic case, the correlation length diverges in the direction (either x or y) in which the coupling becomes stronger. The results are compared with the experimental data on Cs_2CoCl_4. The critical exponents (η',ν') of the correlation function and correlation length are also calculated near the critical temperature ($T=0$) for different anisotropies, and it is found that the system behaves like an Ising model when a little anisotropy is introduced.

I. INTRODUCTION

The study of one-dimensional (1D) spin chains is of growing interest in many-body and condensed-matter physics. This is because exact solutions are comparatively easier in 1D systems than in higher dimensions, and the extensive availability of 1D compounds makes it possible to verify the theoretical predictions in real systems. In this paper we consider an anisotropic spin-$\frac{1}{2}$ XY Hamiltonian which has been exactly solved by Lieb, Schultz, and Mattis.[1] With the help of the Jordan-Wigner transformation they solved the Hamiltonian and calculationed the ground-state correlation functions and formulated the finite-temperature correlation functions. Katsura[2] solved the anisotropic XY model in the presence of a longitudinal magnetic field with the help of the Jordan-Wigner transformation and calculated the thermodynamic properties, e.g., magnetic susceptibility, specific heat, etc. McCoy[3] made calculations of zero- and finite-temperature correlation functions for different anisotropies in the large-N limit. For finite temperatures, he made high- and low-temperature expansions. Tonegawa[4] calculated analytically the correlation functions at $T=0$ for isotropic XY system. At finite temperatures, he calculated numerically the longitudinal as well as transverse spin-correlation functions and the corresponding inverse correlation lengths.

In this paper we have calculated the correlation functions for isotropic as well as anisotropic systems using the method given by Lieb, Schultz, and Mattis[1] and compared with the existing results of McCoy.[3] At finite temperatures, we have calculated the inverse correlation lengths for different anisotropies and explained the experimental data[5] of the compound Cs_2CoCl_4. Cs_2CoCl_4 is a compound which behaves as a linear spin-$\frac{1}{2}$ XY magnetic system.[5-8] The experimentalists[5] obtained the temperature variation of inverse correlation length (κ) from neutron diffraction experiments. They suggest that the observed κ is in reasonable agreement with the temperature dependence of κ_x for an isotropic XY system. The present calculation shows that the experimental κ is an admixture of κ_x and κ_y.

It is evident from our calculation of inverse correlation lengths that at $T=0$, all components of the correlation length diverge for an isotropic system. For an anisotropic system ($\gamma>0$) only the x component diverges. This suggests $T=0$ to be the critical temperature for isotropic as well as anisotropic XY chain. We have, therefore, calculated the critical exponents (ν',η') of correlation length (ξ) and correlation function (ρ) and studied their variation with anisotropy.

II. THEORY

The Hamiltonian of anisotropic linear spin-$\frac{1}{2}$ XY system is given by

$$\mathcal{H}=-2J\sum_{i=1}^{N}[(1+\gamma)S_i^xS_{i+1}^x+(1-\gamma)S_i^yS_{i+1}^y] , \quad (1)$$

where γ is the anisotropy parameter which ranges from 0 to 1. When $\gamma=1$, the Hamiltonian reduces to Ising one.

S_i^x, S_i^y, and S_i^z may be represented by the Pauli spin matrices ($\hbar=1$)

$$S_i^x=\tfrac{1}{2}\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix},\quad S_i^y=\tfrac{1}{2}\begin{bmatrix}0 & -i\\ i & 0\end{bmatrix},\quad S_i^z=\tfrac{1}{2}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix} . \quad (2)$$

Lieb, Schultz, and Mattis[1] solved this model, and they developed a formalism for calculating the correlation functions between two spins. The three components of spin-spin correlations are defined as

$$\rho_n^\alpha=\langle S_i^\alpha S_{i+n}^\alpha\rangle_\beta \quad (\alpha=x,y,z) , \quad (3)$$

where $\beta=1/kT$ and

$$\langle A\rangle_\beta=\frac{\mathrm{Tr}(e^{-\beta\mathcal{H}}A)}{\mathrm{Tr}e^{-\beta\mathcal{H}}} .$$

In the thermodynamic limit ($N \rightarrow \infty$) the expressions of ρ_n^x, ρ_n^y, and ρ_n^z are given[1] as follows:

$$\rho_{2n}^x = \tfrac{1}{4}R_n^2, \quad \rho_{2n-1}^x = \tfrac{1}{4}R_{n-1}R_n \ , \tag{4}$$

where

$$R_n = \begin{vmatrix} G_{-1} & G_{-3} & \cdots & G_{-(2n-1)} \\ G_1 & G_{-1} & \cdots & G_{-(2n-3)} \\ \vdots & \vdots & & \vdots \\ G_{2n-3} & G_{2n-5} & \cdots & G_{-1} \end{vmatrix} . \tag{5}$$

The quantity G_n is defined by

$$G_n = \int_0^{\pi/2} \frac{\cos Kn}{\cos K} \tanh(-J\beta\lambda_K)dK \quad \text{when } n \text{ is odd}$$
$$=0 \quad \text{when } n \text{ is even} \tag{6}$$

and

$$\lambda_K^2 = 1-(1-\gamma^2)\sin^2 K \ . \tag{7}$$

ρ_n^y is obtained if the sign of γ is reversed in the expression of ρ_n^x. The z component of the correlation function is given by

$$\rho_n^z = \tfrac{1}{4}G_n G_{-n} \quad \text{if } n \text{ is odd}$$
$$=0 \quad \text{if } n \text{ is even} \ . \tag{8}$$

Let us define[4] the different components of inverse correlation lengths as

$$\kappa_{x,y} = -\lim_{n\rightarrow\infty} \ln|\rho_{n+1}^{x,y}/\rho_n^{x,y}|$$

and (9)

$$\kappa_z = -\tfrac{1}{2}\lim_{n\rightarrow\infty} \ln(\rho_{2n+3}^z/\rho_{2n+1}^z) \ .$$

For $J>0$ both $\rho_{2n}^{x,y}$ and $\rho_{2n+1}^{x,y}$ (i.e., even and odd correlation functions) have $+ve$ signs but when $J<0$, $\rho_{2n+1}^{x,y}$ changes sign. As defined in Eq. (9) $\kappa_{x,y}$ should not depend on the sign of J.

It has been observed that

$$\kappa_\alpha \rightarrow 0 \text{ as } T\rightarrow 0 \quad (\alpha=x,y,z)$$

and (10)

$$\lim_{n\rightarrow\infty} \rho_n^\alpha = 0 \text{ at } T=0$$

for the isotropic XY system. But for the anisotropic XY system[3] ($\gamma>0$),

$$\kappa_x \rightarrow 0 \quad \text{as } T\rightarrow 0$$

and (11)

$$\lim_{n\rightarrow\infty} \rho_n^x \neq 0 \text{ at } T=0 \ .$$

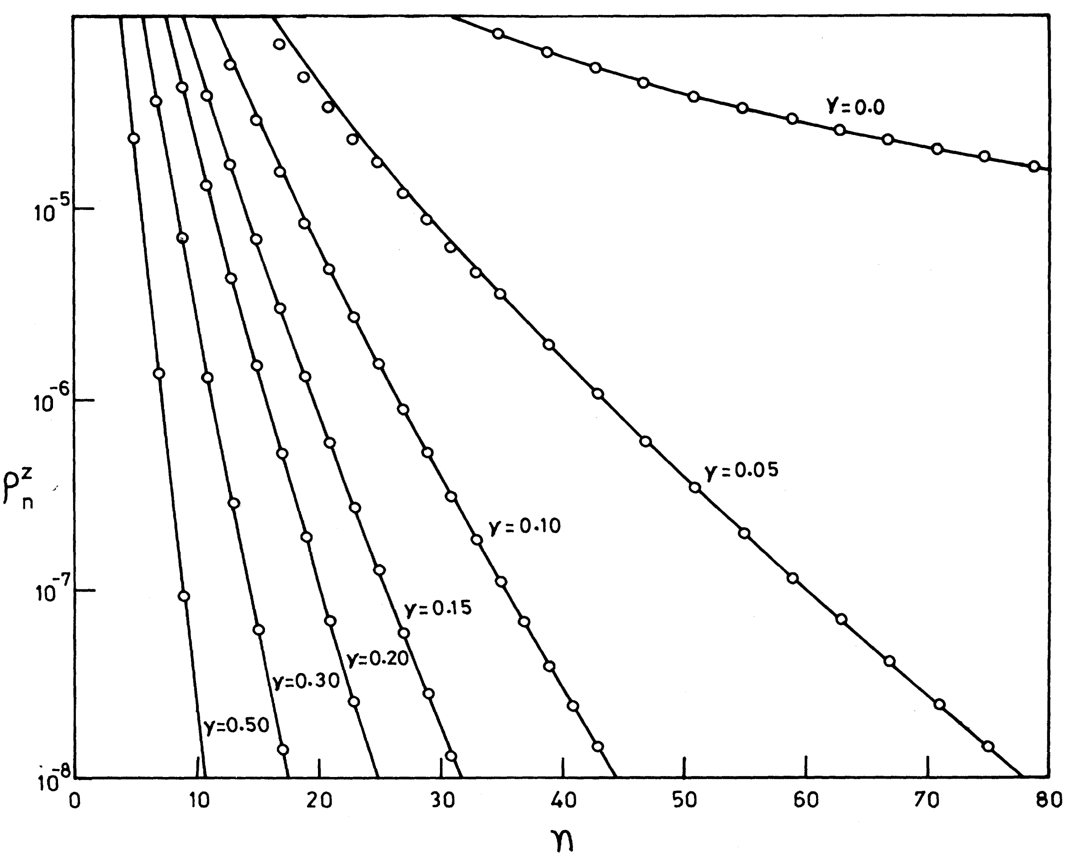

FIG. 1. Ground-state correlation functions in the z direction for different anisotropies. Open circles denote the results of McCoy (Ref. 3).

This means $T=0$ is the critical temperature. Critical exponents (η', ν') are defined as follows.

At the critical temperature $(T=0)$

$$\rho_n \propto n^{-\eta'} \text{ when } n \ll \xi \text{ (the correlation length)} \tag{12}$$

and as $T \to 0$

$$\rho_n \propto e^{-n/\xi} \text{ when } n \gg \xi \,. \tag{13}$$

ξ is a function of temperature. For isotropic XY system[3,4,9] $(\gamma=0)$ at $T=0$

$$\rho_n^x \propto n^{-1/2} \tag{14}$$

for all values of n. Therefore, $\eta'=\frac{1}{2}$ for this system. At the critical point, for general Ising system[10] $(\gamma=1)$,

$$\rho_n \propto n^{2-d-\eta} \tag{15}$$

and for linear Ising system,

$$\rho_n \propto n^{-(\eta-1)} \,. \tag{16}$$

Therefore, $\eta'=\eta-1$ for Ising system in one dimension.

If ν be the critical exponent of correlation length ξ, then

$$\xi \propto t^{-\nu'} \tag{17}$$

where t is the scaling field. For the isotropic XY system[9] $(\gamma=0)$, the temperature (T) is the scaling field and ν' is 1.

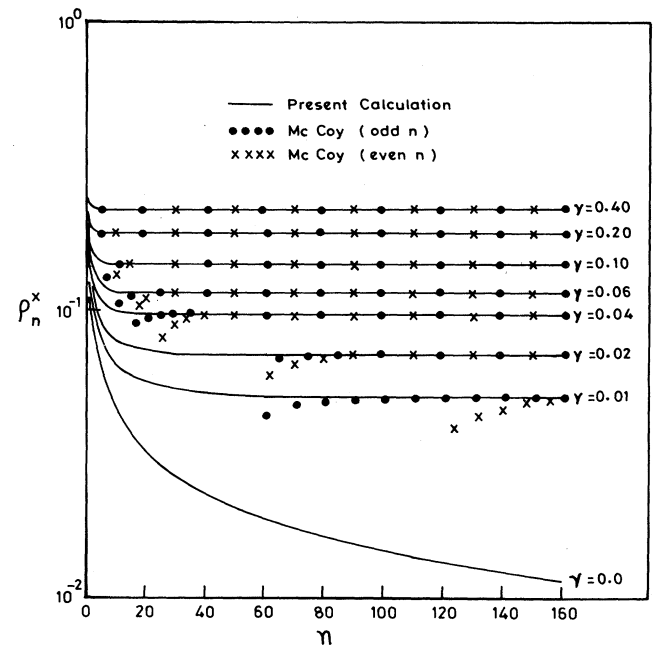

FIG. 2. Ground-state correlation functions in the x direction for different anisotropies. For isotropic case $(\gamma=0)$, McCoy's result (Ref. 3) is four times larger than the present result for all n. The present results, however, agree with the results of Tonegawa (Ref. 4).

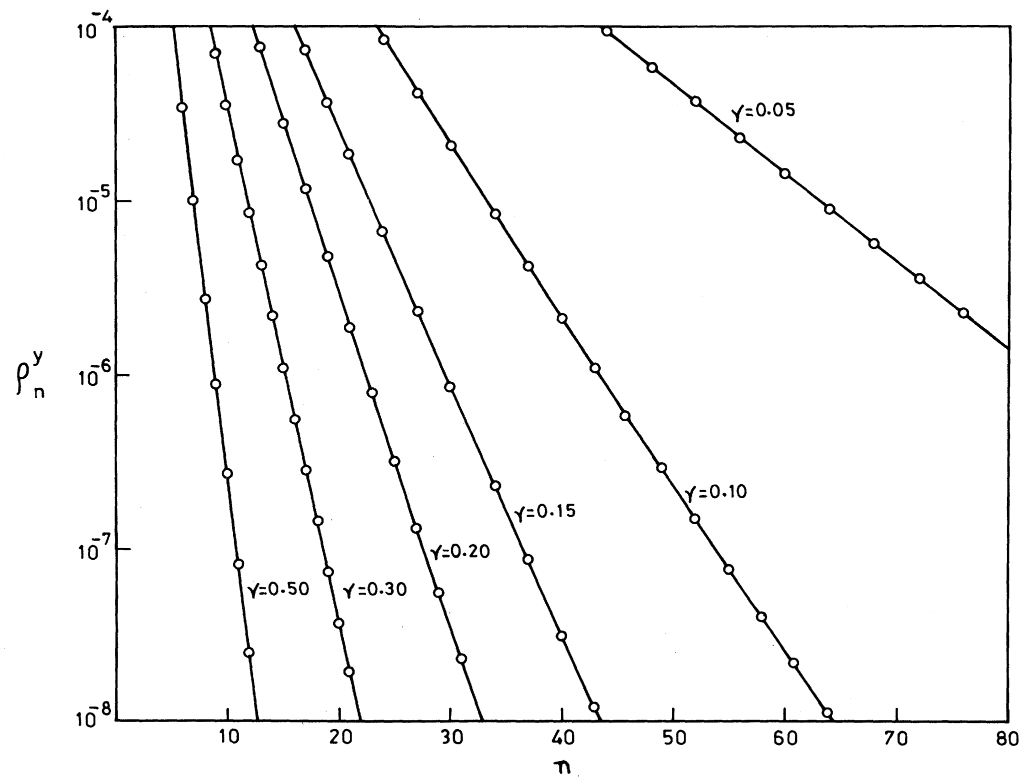

FIG. 3. Ground-state correlation functions in the y direction for different anisotropies. Open circles denote the results of McCoy (Ref. 3).

For the Ising system,[10] $e^{-2J/kT}$ is the scaling field and ν' is 1, where the corresponding Hamiltonian is

$$\mathcal{H}_{\text{Ising}} = -4J \sum_i S_i^z S_{i+1}^z \ . \tag{18}$$

This is the same as the Hamiltonian obtained from Eq. (1) in the Ising limit ($\gamma = 1$).

III. RESULTS AND DISCUSSION

We have computed numerically the correlation functions in x and z directions using Eqs. (4) and (8). The y component of correlation function is obtained if the sign of the anisotropy parameter (γ) is reversed in the expression for ρ_n^x. The zero-temperature results for ρ_n^z, ρ_n^x, and ρ_n^y are shown in Figs. 1, 2, and 3, respectively. In Fig. 1 only odd correlations are shown as even correlations are zero by Eq. (8). We have also evaluated these correlations following McCoy,[3] and they are shown in Figs. 1–3 for comparison. Since McCoy's results are valid for large n, the agreement of our results with those of McCoy is good for large n. As evident from Fig. 2, there is a long-range order in the x direction for the anisotropic system ($\gamma > 0$) since ρ_n^x decays to a constant value as $n \to \infty$. But for isotropic system, no such ordering exists. The y and z components of the correlations go to zero as $n \to \infty$ for both isotropic and anisotropic systems (Figs. 1 and 3). At finite temperatures, we have calculated the inverse correlation lengths (κ) using Eq. (9). The results are plotted in Fig. 4. The value of magnetic exchange interaction in our calculation is $|J|/k = 0.5$ K. We have calculated κ_y and κ_z in the region of n where $\rho_n^{y,z} \sim 10^{-10}$ (lowest reliable number in the computer). At a given temperature, ρ_n^y and ρ_n^z fall sharply and we call the value of n as n_c where the correlation function ($\rho_n^{y,z}$) decays to a value $\sim 10^{-10}$. n_c, however, varies with temperature and anisotropy. ρ_n^x, on the other hand, varies slowly with n and κ_x has been calculated using Eq. (9). This calculation has been performed in the region $n > 100$, since in this region the quantity $|\rho_{n+1}^x / \rho_n^x|$ reaches the convergent limit. It is evident from Fig. 4 that as $T \to 0$, the x component of correlation lengths (ξ_x) diverges for both isotropic and anisotropic systems. On the other hand, the y and z components of correlation length (ξ_y, ξ_z) diverge for the isotropic system only, and they remain finite for the anisotropic system ($\gamma > 0$). As $T \to 0$, the limiting values of κ_y and κ_z are equal, and they agree with the values obtained

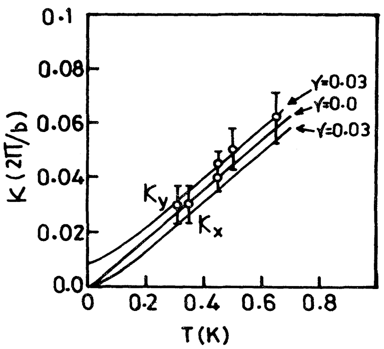

FIG. 5. Experimental results of Cs_2CoCl_4.

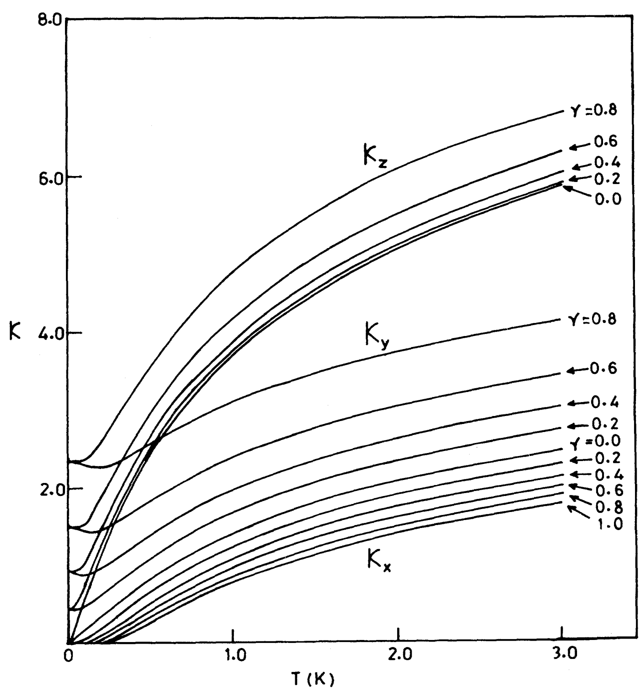

FIG. 4. Temperature variation of inverse correlation lengths in the x, y, z directions.

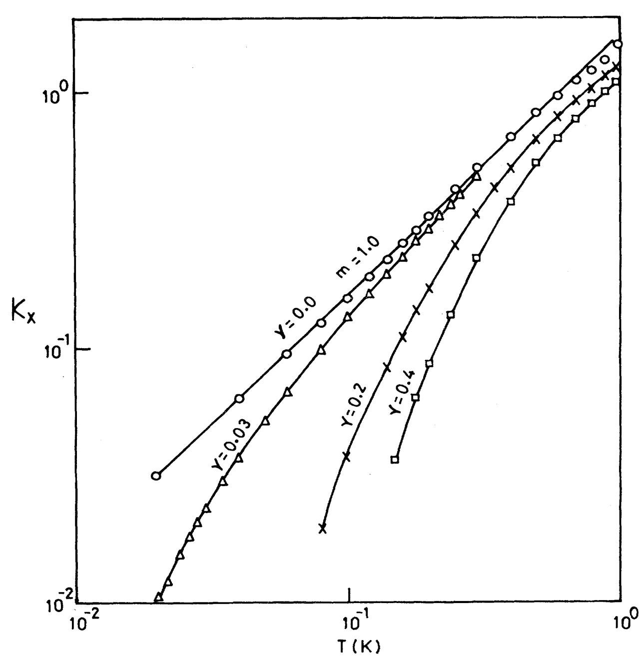

FIG. 6. Calculation of critical exponents ν' when the scaling field is T.

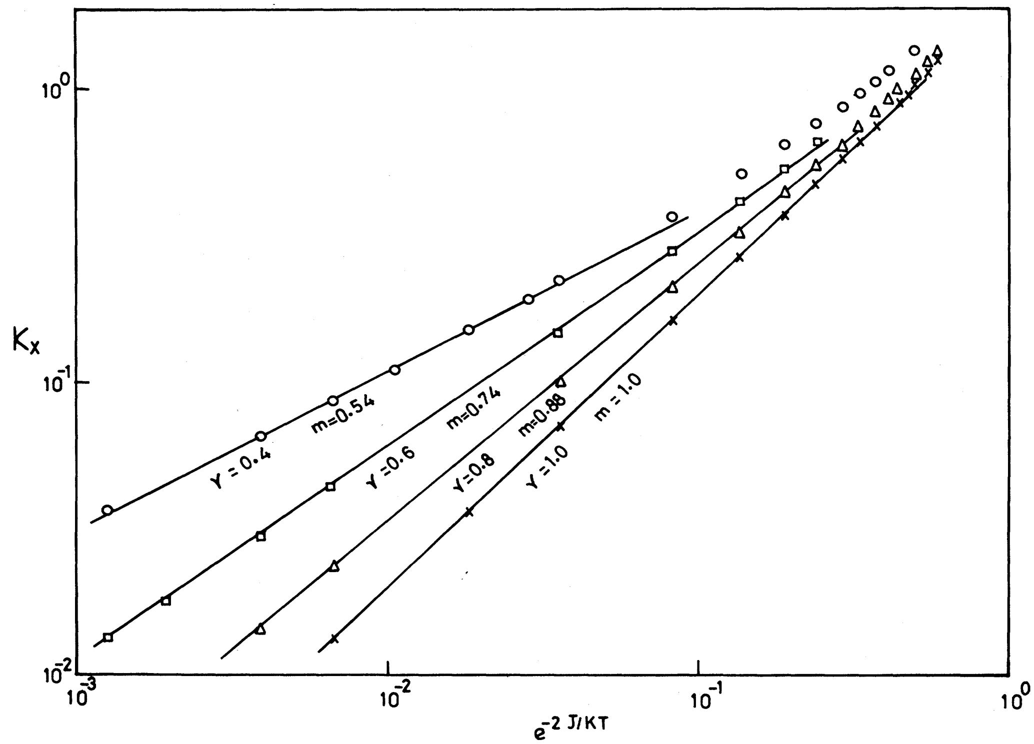

FIG. 7. Calculation of critical exponents ν' assuming $e^{-2J/kT}$ to be the scaling field.

by McCoy.[3] When $\gamma=1.0$, in both y and z directions, autocorrelations only exist and other correlations vanish. As a result, $\gamma=1.0$ case has been omitted in Fig. 4 for y and z components.

We have applied our calculations to explain the magnetic behavior of Cs_2CoCl_4. Recent measurements of heat capacity[6] and susceptibility[7,8] suggest that the compound might be 1D XY antiferromagnetic in nature. The magnetic behavior of this compound has also been studied by quasielastic neutron scattering techniques.[5] A sheetlike structure in the static correlation function expresses the 1D nature of the compound. From the experimental data, the temperature variation of inverse correlation length (κ) was obtained. The experimentalists[5] compared their results with those of linear isotropic XY model as obtained by Tonegawa.[4] They suggested that the results are in reasonable agreement with the temperature dependence of κ_x of the 1D XY model. They also showed that the possibility of mixing of κ_z is negligible. Here we have calculated both κ_x and κ_y for $\gamma=0.03$ and compared with the experimental results as shown in Fig. 5. The results of κ_x (or κ_y) for the isotropic XY ($\gamma=0$) system has been plotted in this figure for comparison. The value of exchange interaction to compare the experimental results[5] is $|J|/k=1.47$ K which is same as to interpret the specific-heat data.[6] It is evident from Fig. 5 that the experimental results of κ may be an admixture of κ_x and κ_y with small amount of anisotropy ($\gamma=0.03$).

The study of correlation functions and inverse correlation lengths discussed so far leads to an important fact that as $T\to 0$, the correlation length diverges in all directions for isotropic system ($\gamma=0$), and in the x direction only for anisotropic system ($\gamma>0$). Therefore, $T=0$ is the critical temperature for isotropic as well as anisotrop-

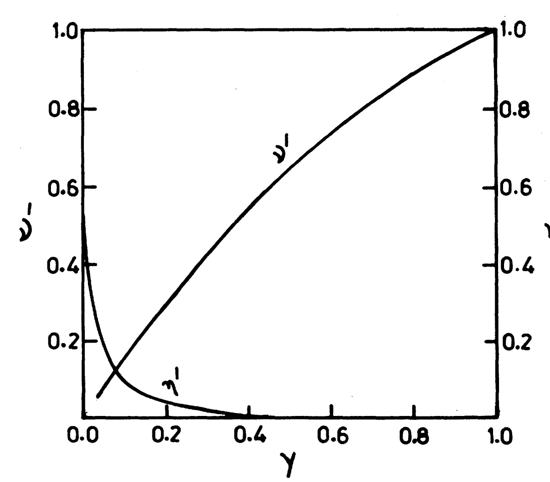

FIG. 8. Variation of critical exponents (ν',η') with anisotropy (γ).

ic XY systems, and it is interesting to calculate the effective critical exponents (ν', η') for such systems.

At $T=0$, we have observed that in the low-n region, ρ_n^x follows power law decay as $\rho_n^x \sim n^{-\eta}$. If ρ_n^x is plotted against n in a double log scale, we get a straight line, the slope of which determines the value of η'. For the isotropic XY system $(\gamma=0)$ $\eta'=\frac{1}{2}$ and for the Ising system $(\gamma=1)$ $\eta'=0$ as ρ_n^x remains constant with the increase of n. These values are same as obtained analytically by McCoy.[3]

We have also calculated the critical exponents (ν') of correlation length (ξ) about $T=0$. For the isotropic XY system the scaling field[9] is T. In Fig. 6 the calculated values of κ_x for isotropic and three different anisotropic systems are plotted against T in a double-log scale. The $\gamma=0$ curve shows a straight-line behavior near $T=0$ and the slope (m) gives the critical exponent $\nu'=1$. From this figure, it is evident that if a small anisotropy is introduced, the curve continuously bends, and no straight-line characteristic is obtained in the low-temperature region. This is probably because T is not the proper scaling field for the anisotropic XY system. For Ising system, the scaling field[10] is $e^{-2J/kT}$ corresponding to the Hamiltonian $\mathcal{H}=-4J\sum_i S_i^z S_{i+1}^z$. The Hamiltonian of our system [Eq. (1)] reduces to an Ising one when $\gamma=1.0$. Therefore, for anisotropic system $(\gamma>0)$, we use $e^{-2J/kT}$ as the scaling field to calculate the critical exponents (ν') of correlation length (ξ).

In our calculations, the value of exchange interaction is taken to be $|J|/k=0.5$ K and the value of κ_x will be same for both ferromagnetic and antiferromagnetic interaction as followed by Eq. (9). Therefore, the scaling field t for the ferromagnetic case will be $e^{-2J/kT}=e^{-1/T}$. In Fig. 7 we have plotted the results of κ_x against t $(=e^{-1/T})$ in a double-log scale for different values of anisotropy. For each anisotropy, a good straight line curve is obtained in the low-temperature region. The slope (m) of these straight lines determines the value of the exponents ν'. It has been observed that the low-temperature data for $\gamma=0.03$ (Fig. 6) if plotted against the scaling field $e^{-2J/kT}$ gives a straight line, and it is possible to calculate the effective critical exponent (ν'). These effective exponents are, however, functions of the anisotropy parameter (γ) and their variations with the anisotropy parameter (γ) are shown in Fig. 8. As shown in Fig. 8, the exponents (ν', η') in the Ising limit $(\gamma=1)$ are recovered from these curves. In the isotropic XY limit $(\gamma=0)$, although the value of the exponent η is recovered, that of ν is not, because the scaling field changes from $e^{-2J/kT}$ to T in this limit.

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