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# The exact solution of magnetic susceptibility for finite Ising ring with a magnetic impurity

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## Abstract

We connected the two ends of a finite spin-1/2 antiferromagnetic Ising chain with a magnetic impurity at one end to form a closed ring, and studied the magnetic susceptibility of it exactly by using the transfer matrix method. We calculated the magnetic susceptibility in the whole temperature range and gave the phase diagram at ground state of the system about the anisotropy of the impurity and strength of the connection exchange interaction for spin-1 and 3/2 impurities. We also gave the ground state entropy of system and derived the asymptotic expression of the magnetic susceptibility multiplied by temperature at zero temperature limit and high temperature limit. It is found that degenerate phase may exist in some parameter region at zero temperature for the spin number of system being odd, and the ground state entropy is  $\ln(2)$  in the nondegenerate phase and is dependent on the number of spin in the degenerate phase. The magnetic susceptibility of the system at low temperature exhibits ferromagnetic behavior, and the Curie constant is related to the spin configuration at ground state. When the ground state is nondegenerate, the Curie

constant is equal to the square of the net spin, regardless of the parity of the number of the spin. When the number of spin is odd and the ground state is degenerate, the Curie constant may be related to the total number of spin. In high temperature limit, the magnetic susceptibility multiplied by temperature is related to the spin quantum number of impurity and the number of spin in the ring.

**Keywords: transfer matrix method, magnetic susceptibility, magnetic impurity, Ising ring, Curie's law**

## 1. Introduction

In condensed matter physics, the variants of low dimensional quantum antiferromagnetic system have received much attention due to its low dimensionality and novel phenomenon arising from the quantum fluctuations[1,2]. In theory, The magnetic properties of antiferromagnetic chain with impurity have been widely studied. It is found that the result of the convergence of magnetic susceptibility for antiferromagnetic chain decorated with spin pendant in the low temperature is very different from that of the pure antiferromagnetic chain [1]. The magnetic susceptibility of antiferromagnetic chain with ferromagnetic sawteeth (Delta chain) shows Curie law behavior at low temperature, the Curie constant in zero temperature limit is related to the degeneracy of the system, and the specific heat in the ultra-low temperature shows obvious size effect [2]. By doping impurities, an antiferromagnetic spin chain can be divided into many finite parts, thus the boundary effect on the magnetic behavior of the system may appear. For example, in a finite anisotropic Heisenberg antiferromagnetic chain, it is discovered that the magnetic susceptibility multiplied by temperature in low temperature is related to the length of the chain[3]. In the semi-infinite XXZ antiferromagnetic chain, the boundary magnetic susceptibility of system shows divergence in zero temperature limit[4]. In a finite Ising antiferromagnetic chain with a impurity at one end, the magnetic susceptibility multiplied by temperature in zero temperature limit is found proportional to the square of net spin and has nothing to do with the value of the impurity anisotropy and the exchange interaction between impurity and the host[5]. For a part of

antiferromagnetic chain, the behavior of the magnetic susceptibility in low temperature is found to be related to the parity of the number of the spin and the defect position[6,7]. When the two dimensional antiferromagnet is doped by defects or impurities, the susceptibility of system in low temperature limit shows some abnormal behaviors[8,9]. And for the mixed-spin bathroom tile lattice, the magnetization was found to be influenced by the spin quantum number and single-ion anisotropy strength[10].

Experiments indeed found the effect of the magnetic or nonmagnetic impurity on the antiferromagnet. The quasi one-dimensional  $\text{Cu}_2\text{MSiO}_5$  ( $M = \text{Co}, \text{Ni}$ ) antiferromagnet synthesized recently, doped Co or Ni, shows different magnetic susceptibility in low temperature[11]. As the Co ion in the low-dimensional  $\text{CoTa}_2\text{O}_6$  antiferromagnet is replaced by Mg ion to an extent, the ferromagnetic behavior of the system in the low temperature can be explained by the anisotropic Heisenberg model or Ising model[12]. In quasi one-dimensional  $\text{Sr}_2\text{CuO}_3$  antiferromagnet, it is found that the external magnetic field can induce the local magnetic moment near the nonmagnetic impurity, and local magnetic susceptibility shows a high peak in the low temperature, reflecting the obvious ferromagnetic characteristics and confirmed by theory[3,13,14]. Doping Mg ion into one-dimensional  $\text{SrCuO}_2$  antiferromagnetic chain to get  $\text{SrCu}_{1-x}\text{Mg}_x\text{O}_2$  chain, the magnetic susceptibility of the system in low temperature converges to different finite values when x get different value[15].

In many low-dimensional antiferromagnets, the energy of each bond cannot reach the minimum at the same time due to the geometric structure, this is the

so-called frustration phenomenon, such as Delta chain and the triangle structure in azurite and in  $K_2MnS_{2-x}Se_x$ [2,16-19]. Because of the energy gap between the ground state and the excited state, the specific heat of the frustrated system usually shows peak in the low temperature, and the magnetic susceptibility is also different from that of antiferromagnetic system without frustration [17-19]. If we connect the two ends of the finite antiferromagnetic spin chain with an impurity through antiferromagnetic interaction to form a closed ring, the boundary effect may be eliminated, but it will bring geometric frustration effect when the number of spin is odd. The behavior of the magnetic susceptibility of the system compared with the open chain is worth studying [5]. In two-ring structure [19], multi-ring structure[20] and Ising-Heisenberg diamond chain[21], the specific heat and susceptibility are found to show double peaks with temperature in some parameter range. For the Ising and Ising-like models, the approximate and exact solution have been given in the reference[22].

In this paper we will study the finite length defective antiferromagnetic Ising closed ring. Using the transfer matrix method[5,6,22,23], we will calculate exactly the magnetic susceptibility of the system, and discuss the effect of impurity anisotropy, host-impurity exchange interaction, and spin quantum number of impurity on the magnetic susceptibility. The arrangement of the paper is as follows: Sec. II presents the exact solution for the finite spin-1/2 Ising ring with a magnetic impurity. In Sec. III we describe its ground-state properties, and the behavior of magnetic susceptibility, especially the value in the zero temperature limit. In Sec. IV we make a brief summary.

## 2. model and method

We set up a spin-1/2 antiferromagnetic finite Ising ring by connecting the two ends of a Ising chain with a impurity on one end,  $S_i^Z$  denotes the host spin,  $\mu_N^Z$  represents the magnetic impurity spin at site  $N$ , as shown in Fig.1. The Hamiltonian is given by,

$$H = J \sum_{i=1}^{N-2} S_i^Z S_{i+1}^Z + JS_{N-1}^Z \mu_N^Z + J_1 \mu_N^Z S_1^Z - h \sum_{i=1}^{N-1} S_i^Z - h \mu_N^Z - D(\mu_N^Z)^2 \quad (1)$$

where  $S_i^Z = \pm \frac{1}{2}$ , and  $\mu_N^Z = -1, 0, 1$  or  $-\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}$ , representing the impurity spin state with spin quantum number  $\mu_N$  of 1 or 3/2 respectively. The host-impurity exchange interaction (connecting exchange interaction) is  $J_1$  at the closed place, and the other antiferromagnetic exchange interaction between the nearest-neighbor spins is  $J$ .  $D$  is the single-ion anisotropy of the impurity, and  $h$  is the external magnetic field.

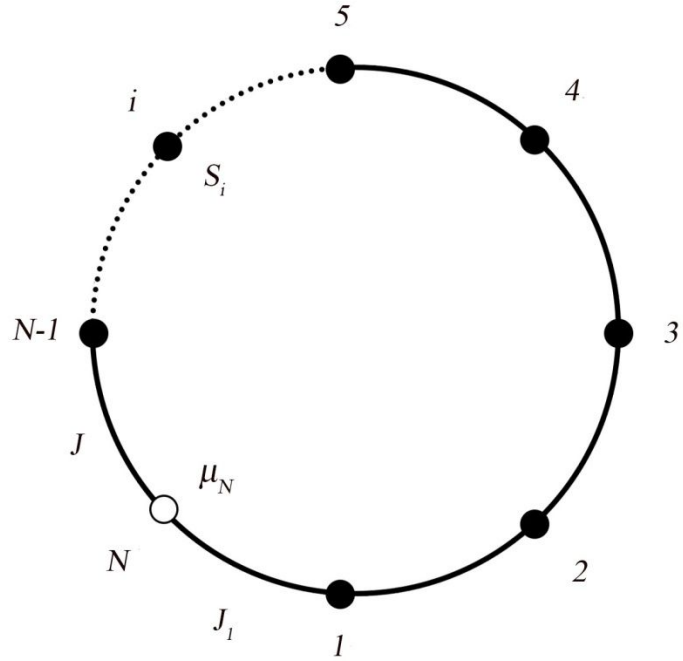


Fig.1. Antiferromagnetic Ising spin ring with a impurity spin at site N.

By using the transfer matrix method, the partition function of the system can be expressed as follow,

$$Z = \text{Tr}(e^{-\beta H}) = \text{Tr}(\mathbf{P}^{N-2} \mathbf{P}_1 \mathbf{P}_2) \quad (2)$$

here  $\beta = 1/(k_B T)$  and the matrix elements of  $\mathbf{P}$ ,  $\mathbf{P}_1$  and  $\mathbf{P}_2$  are given respectively by,

$$P_{S_i^z, S_{i+1}^z} = e^{-\beta(J S_i^z S_{i+1}^z - \frac{1}{2} h (S_i^z + S_{i+1}^z))} \quad (3a)$$

$$P_{1 S_{N-1}^z, \mu_N^z} = e^{-\beta(J S_{N-1}^z \mu_N^z - \frac{1}{2} h (S_{N-1}^z + \mu_N^z) - \frac{1}{2} D (\mu_N^z)^2)} \quad (3b)$$

$$P_{2 \mu_N^z, S_1^z} = e^{-\beta(J_1 \mu_N^z S_1^z - \frac{1}{2} h (\mu_N^z + S_1^z) - \frac{1}{2} D (\mu_N^z)^2)} \quad (3c)$$

By introducing the unitary matrix  $\mathbf{V}$ , we can diagonalize the matrix  $\mathbf{P}$ , thus the partition function is written as,

$$Z = \text{Tr}(\boldsymbol{\lambda}^{N-2} \mathbf{V}^{-1} \mathbf{P}_1 \mathbf{P}_2 \mathbf{V}) = \lambda_1^{N-2} R_{11} + \lambda_2^{N-2} R_{22} \quad (4)$$

and the entropy of system can be given by,



$$S = k_B \ln(Z) + k_B T \frac{\partial \ln(Z)}{\partial T} \quad (5)$$

where  $\mathbf{V}^{-1}$  is the inverse matrix of matrix  $\mathbf{V}$ ,  $\boldsymbol{\lambda}$  is a diagonal matrix,

$$\boldsymbol{\lambda} = \mathbf{V}^{-1} \mathbf{P} \mathbf{V} = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} \quad (6)$$

$$\mathbf{R} = \mathbf{V}^{-1} \mathbf{P}_1 \mathbf{P}_2 \mathbf{V} = \begin{pmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{pmatrix} \quad (7)$$

here[5],

$$\lambda_{1,2} = e^{-\frac{1}{4}\beta J} \cosh\left(\frac{1}{2}\beta h\right) \pm \sqrt{e^{-\frac{1}{2}\beta J} \sinh^2\left(\frac{1}{2}\beta h\right) + e^{\frac{1}{2}\beta J}} \quad (8)$$

$$\mathbf{V} = \begin{pmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{pmatrix} \quad (9)$$

with

$$V_{11} = \frac{1}{\sqrt{1 + \left(\lambda_1 e^{-\frac{1}{4}\beta J} - e^{-\frac{1}{2}\beta(J-h)}\right)^2}}$$

$$V_{12} = \frac{1}{\sqrt{1 + \left(\lambda_2 e^{-\frac{1}{4}\beta J} - e^{-\frac{1}{2}\beta(J-h)}\right)^2}}$$

$$V_{21} = \frac{\left(\lambda_1 e^{-\frac{1}{4}\beta J} - e^{-\frac{1}{2}\beta(J-h)}\right)}{\sqrt{1 + \left(\lambda_1 e^{-\frac{1}{4}\beta J} - e^{-\frac{1}{2}\beta(J-h)}\right)^2}}$$

$$V_{22} = \frac{\left(\lambda_2 e^{-\frac{1}{4}\beta J} - e^{-\frac{1}{2}\beta(J-h)}\right)}{\sqrt{1 + \left(\lambda_2 e^{-\frac{1}{4}\beta J} - e^{-\frac{1}{2}\beta(J-h)}\right)^2}}$$

The magnetization  $m$  per spin of the system is defined as,

$$m = \frac{\langle M \rangle}{N} = \frac{1}{N} \left\langle \left( \sum_{i=1}^{N-1} S_i^z + \mu_N^z \right) \right\rangle$$

(10)

The magnetic susceptibility of system,  $\chi = \left. \frac{\partial \langle M \rangle}{\partial h} \right|_{h=0}$ ,

$$\chi = \frac{1}{k_B T} (\langle MM \rangle - \langle M \rangle \langle M \rangle) \quad (11)$$

When the external magnetic field  $h$  is 0, the magnetization  $m$  of the system is 0, thus

$$\langle M \rangle = 0$$

The magnetic susceptibility multiplied by temperature becomes,

$$\chi T = \left\langle \left( \sum_{i=1}^{N-1} S_i^Z + \mu_N^Z \right) \left( \sum_{i=1}^{N-1} S_i^Z + \mu_N^Z \right) \right\rangle \quad (12)$$

here we take the Boltzmann's constant  $k_B = 1$  .

The right hand of Equation (12) can be divided into single-point correlation function  $F1$  and two-points correlation function  $F2$ , where

$$F1 = \langle (S_1^Z)^2 + (S_2^Z)^2 + (S_3^Z)^2 + \dots + (S_{N-1}^Z)^2 + (\mu_N^Z)^2 \rangle \quad (13)$$

$$\begin{aligned} F2 = & 2 \langle S_1^Z S_2^Z + S_1^Z S_3^Z + S_1^Z S_4^Z + \dots + S_1^Z S_{N-1}^Z + S_1^Z \mu_N^Z \rangle \\ & + 2 \langle S_2^Z S_3^Z + S_2^Z S_4^Z + \dots + S_2^Z S_{N-1}^Z + S_2^Z \mu_N^Z \rangle \\ & + \dots \\ & + 2 \langle S_{N-2}^Z S_{N-1}^Z + S_{N-2}^Z \mu_N^Z \rangle \\ & + 2 \langle S_{N-1}^Z \mu_N^Z \rangle \end{aligned} \quad (14)$$

By using transfer matrix method, single-point correlation function  $F1$  can be written as,

$$\begin{aligned}
F1 &= \left\langle \frac{N-1}{4} + (\mu_N^Z)^2 \right\rangle \\
&= \frac{N-1}{4} + \frac{1}{Z} \text{Tr}(\mathbf{P}^{N-2} \mathbf{V}^{-1} \mathbf{P}_1 (\mu_N^Z)^2 \mathbf{P}_2 \mathbf{V}) \\
&= \frac{N-1}{4} + \frac{\lambda_1^{N-2} Q_{11} + \lambda_2^{N-2} Q_{22}}{\lambda_1^{N-2} R_{11} + \lambda_2^{N-2} R_{22}}
\end{aligned} \tag{15}$$

where,

$$\mathbf{Q} = \mathbf{V}^{-1} \mathbf{P}_1 (\mu_N^Z)^2 \mathbf{P}_2 \mathbf{V} = \begin{pmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{pmatrix} \tag{16}$$

where  $\mu_N^Z$  is a diagonal matrix whose eigenvalues are the diagonal elements,

$$\mu_N^Z = \begin{pmatrix} \mu_N & 0 & 0 & 0 & 0 \\ 0 & (\mu_N - 1) & 0 & 0 & 0 \\ 0 & 0 & \ddots & 0 & 0 \\ 0 & 0 & 0 & -(\mu_N - 1) & 0 \\ 0 & 0 & 0 & 0 & -\mu_N \end{pmatrix} \tag{17}$$

In the zero temperature limit  $T \rightarrow 0$ , the matrix  $\mathbf{V}$  can be simplified as,

$$\mathbf{V} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \tag{18}$$

Thus the diagonal matrix  $\mathbf{S}_i^Z$

$$\mathbf{S}_i^Z = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix} \tag{19}$$

can be transformed to a new diagonal form,

$$\begin{aligned}
&\mathbf{V}^{-1} \mathbf{S}_i^Z \mathbf{V} \lambda^k \mathbf{V}^{-1} \mathbf{S}_j^Z \mathbf{V} \\
&= \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \lambda_1^k & 0 \\ 0 & \lambda_2^k \end{pmatrix} \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\
&= \frac{1}{4} \begin{pmatrix} \lambda_2^k & 0 \\ 0 & \lambda_1^k \end{pmatrix}
\end{aligned} \tag{20}$$

Any term in two-points correlation function  $F2$  can be written as,

$$\begin{aligned}
& \langle S_i^Z S_{i+1}^Z + S_i^Z S_{i+2}^Z + S_i^Z S_{i+3}^Z + \dots + S_i^Z S_{N-1}^Z + S_i^Z \mu_N^Z \rangle \\
&= \frac{1}{Z} \text{Tr}(\mathbf{P}^{i-1} \mathbf{S}_i^Z \mathbf{P} \mathbf{S}_{i+1}^Z \mathbf{P}^{N-3-(i-1)} \mathbf{P}_1 \mathbf{P}_2 + \mathbf{P}^{i-1} \mathbf{S}_i^Z \mathbf{P}^2 \mathbf{S}_{i+2}^Z \mathbf{P}^{N-4-(i-1)} \mathbf{P}_1 \mathbf{P}_2 \\
&+ \mathbf{P}^{i-1} \mathbf{S}_i^Z \mathbf{P}^3 \mathbf{S}_{i+3}^Z \mathbf{P}^{N-5-(i-1)} \mathbf{P}_1 \mathbf{P}_2 + \dots + \mathbf{P}^{i-1} \mathbf{S}_i^Z \mathbf{P}^{N-2-(i-1)} \mathbf{S}_{N-1}^Z \mathbf{P}_1 \mathbf{P}_2 \\
&+ \mathbf{P}^{i-1} \mathbf{S}_i^Z \mathbf{P}^{N-2-(i-1)} \mathbf{P}_1 \mu_N^Z \mathbf{P}_2) \\
&= \frac{1}{Z} \text{Tr}(\lambda^{i-1} \mathbf{V}^{-1} \mathbf{S}_i^Z \mathbf{V} \lambda \mathbf{V}^{-1} \mathbf{S}_{i+1}^Z \mathbf{V} \lambda^{N-3-(i-1)} \mathbf{R} + \lambda^{i-1} \mathbf{V}^{-1} \mathbf{S}_i^Z \mathbf{V} \lambda^2 \mathbf{V}^{-1} \mathbf{S}_{i+2}^Z \mathbf{V} \lambda^{N-4-(i-1)} \mathbf{R} \\
&+ \lambda^{i-1} \mathbf{V}^{-1} \mathbf{S}_i^Z \mathbf{V} \lambda^3 \mathbf{V}^{-1} \mathbf{S}_{i+3}^Z \mathbf{V} \lambda^{N-5-(i-1)} \mathbf{R} + \dots \\
&+ \lambda^{i-1} \mathbf{V}^{-1} \mathbf{S}_i^Z \mathbf{V} \lambda^{N-2-(i-1)} \mathbf{V}^{-1} \mathbf{S}_{N-1}^Z \mathbf{V} \mathbf{R} \\
&+ \lambda^{i-1} \mathbf{V}^{-1} \mathbf{S}_i^Z \mathbf{V} \lambda^{N-2-(i-1)} \mathbf{V}^{-1} \mathbf{P}_1 \mu_N^Z \mathbf{P}_2 \mathbf{V}) \\
&= \frac{1}{Z} \text{Tr} \left( \begin{pmatrix} \frac{1}{4} \lambda_1^{N-3} \lambda_2 R_{11} & 0 \\ 0 & \frac{1}{4} \lambda_1 \lambda_2^{N-3} R_{22} \end{pmatrix} + \begin{pmatrix} \frac{1}{4} \lambda_1^{N-4} \lambda_2^2 R_{11} & 0 \\ 0 & \frac{1}{4} \lambda_1^2 \lambda_2^{N-4} R_{22} \end{pmatrix} + \dots \right. \\
&+ \begin{pmatrix} \frac{1}{4} \lambda_1^{i-1} \lambda_2^{N-2-(i-1)} R_{11} & 0 \\ 0 & \frac{1}{4} \lambda_1^{N-2-(i-1)} \lambda_2^{(i-1)} R_{22} \end{pmatrix} \\
&+ \left. \begin{pmatrix} \frac{1}{2} \lambda_1^{i-1} \lambda_2^{N-2-(i-1)} Y_{21} & 0 \\ 0 & \frac{1}{2} \lambda_1^{N-2-(i-1)} \lambda_2^{(i-1)} Y_{12} \end{pmatrix} \right) \\
&= \frac{1}{\lambda_1^{N-2} R_{11} + \lambda_2^{N-2} R_{22}} \left[ \frac{\frac{1}{4} \lambda_1^{N-3} \lambda_2 \left( 1 - \left( \frac{\lambda_2}{\lambda_1} \right)^{N-2-(i-1)} \right)}{1 - \frac{\lambda_2}{\lambda_1}} R_{11} \right. \\
&+ \frac{\frac{1}{4} \lambda_1 \lambda_2^{N-3} \left( 1 - \left( \frac{\lambda_1}{\lambda_2} \right)^{N-2-(i-1)} \right)}{1 - \frac{\lambda_1}{\lambda_2}} R_{22} \\
&+ \left. \frac{1}{2} \lambda_1^{i-1} \lambda_2^{N-2-(i-1)} Y_{21} + \frac{1}{2} \lambda_1^{N-2-(i-1)} \lambda_2^{(i-1)} Y_{12} \right]
\end{aligned} \tag{21}$$

where,  $i = 1, 2, \dots, N-1$ , the matrix  $\mathbf{Y}$  is defined as,

$$\mathbf{Y} = \mathbf{V}^{-1} \mathbf{P}_1 \boldsymbol{\mu}_N \mathbf{P}_2 \mathbf{V} = \begin{pmatrix} Y_{11} & Y_{12} \\ Y_{21} & Y_{22} \end{pmatrix} \quad (22)$$

By summation of the correlation function of spins,  $F1$  and  $F2$ , we can get

$$\begin{aligned} \lim_{T \rightarrow 0} \chi^T &= \frac{1}{R_{11} + \left(\frac{\lambda_2}{\lambda_1}\right)^{N-2}} \left( \frac{1}{2} \frac{\left( \frac{\lambda_2}{\lambda_1} \left( (N-2) - \frac{\frac{\lambda_2}{\lambda_1} \left( 1 - \left(\frac{\lambda_2}{\lambda_1}\right)^{N-2} \right)}{1 - \frac{\lambda_2}{\lambda_1}} \right) \right)}{1 - \frac{\lambda_2}{\lambda_1}} \right) R_{11} + \frac{1}{2} \\ &\left( \frac{\left(\frac{\lambda_2}{\lambda_1}\right)^{N-3} \left( (N-2) - \frac{\frac{\lambda_1}{\lambda_2} \left( 1 - \left(\frac{\lambda_1}{\lambda_2}\right)^{N-2} \right)}{1 - \frac{\lambda_1}{\lambda_2}} \right)}{1 - \frac{\lambda_1}{\lambda_2}} \right) R_{22} + \left( \frac{\left( 1 - \left(\frac{\lambda_2}{\lambda_1}\right)^{N-1} \right)}{1 - \frac{\lambda_2}{\lambda_1}} \right) Y_{12} \\ &+ \left( \frac{\left(\frac{\lambda_2}{\lambda_1}\right)^{N-2} \left( 1 - \left(\frac{\lambda_1}{\lambda_2}\right)^{N-1} \right)}{1 - \frac{\lambda_1}{\lambda_2}} \right) Y_{21} \\ &+ \left. Q_{11} + \left(\frac{\lambda_2}{\lambda_1}\right)^{N-2} Q_{22} + \frac{N-1}{4} \left( R_{11} + \left(\frac{\lambda_2}{\lambda_1}\right)^{N-2} R_{22} \right) \right\} \quad (23) \end{aligned}$$

In high temperature limit  $T \rightarrow \infty$ , the matrix  $\mathbf{V}$  also satisfy the eq.(18), therefore the form of the  $\chi^T$  in eq. (23) still holds. By using  $\lambda_1 = 2$ ,  $\lambda_2 = 0$ ,  $Y_{12} = 0$ ,  $Y_{21} = 0$

and when  $\mu_N = 1$ ,  $R_{11} = 3$ ,  $Q_{11} = 2$ , when  $\mu_N = \frac{3}{2}$ ,  $R_{11} = 4$ ,  $Q_{11} = 5$ . The  $\chi T$  can be written as,

$$\lim_{T \rightarrow \infty} \chi T = \frac{N-1}{4} + \frac{Q_{11}}{R_{11}} = \begin{cases} \frac{3N+5}{12}, & (\mu_N = 1) \\ \frac{N+4}{4}, & (\mu_N = \frac{3}{2}) \end{cases} \quad (24)$$

In the following section, we will give the magnetic susceptibility of system for different parameter of system and temperature. For convenience, the single-ion anisotropy  $D$ , host-impurity exchange interaction  $J_1$ , temperature  $T$  and external magnetic field  $h$  are reduced by  $J(D \Rightarrow D/J, J_1 \Rightarrow J_1/J, T \Rightarrow T/J, h \Rightarrow h/J)$

### 3. Results and discussions

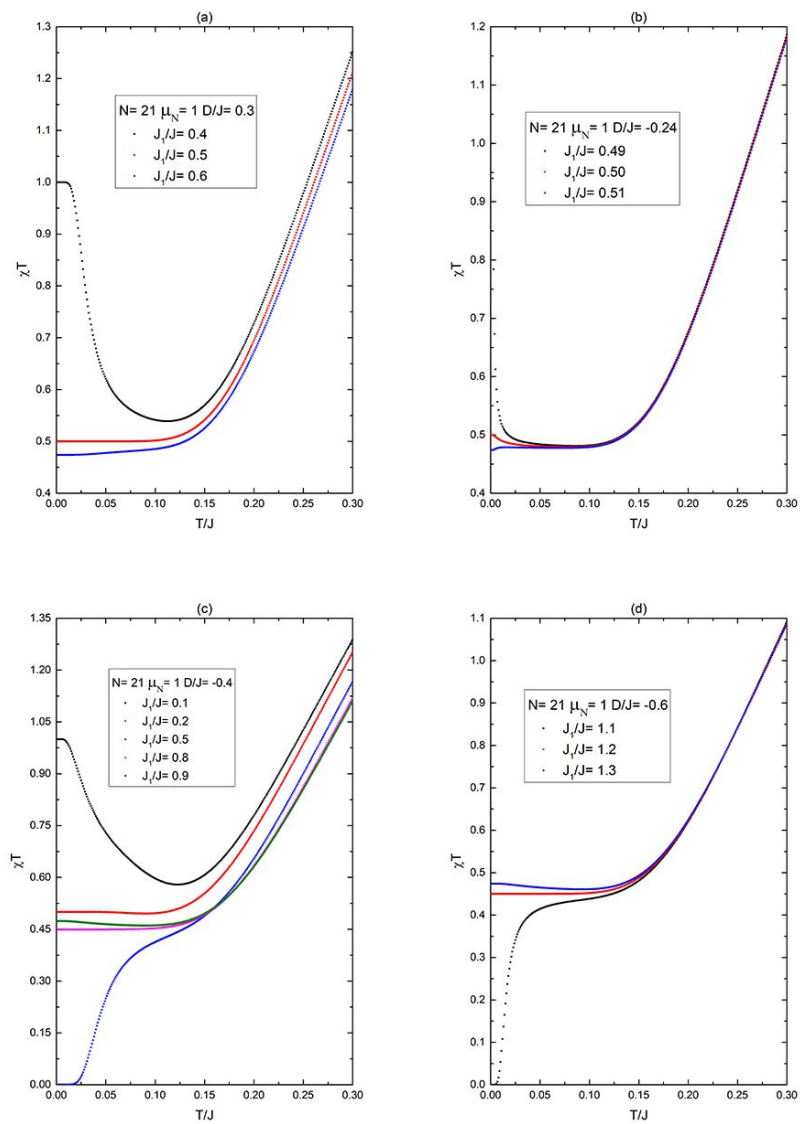


Fig.2. The temperature dependence of  $\chi T$  for different anisotropy of impurity and host-impurity exchange interaction.  $N = 21, \mu_N = 1$ . (a)  $D/J = 0.3$ , (b)  $D/J = -0.24$ , (c)  $D/J = -0.4$ , (d)  $D/J = -0.6$ .

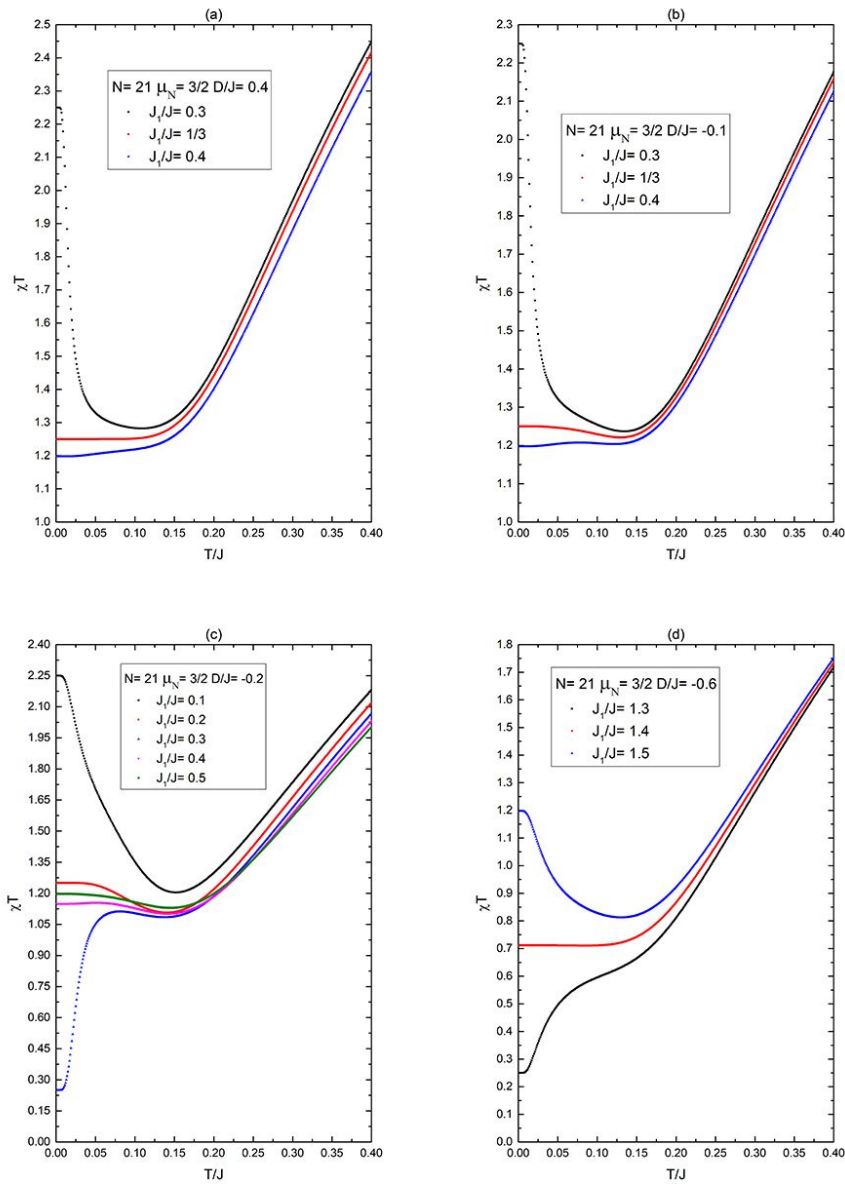


Fig.3. The temperature dependence of  $\chi T$  for different anisotropy of impurity and host-impurity exchange interaction.  $N = 21, \mu_N = 3/2$ . (a)  $D/J = 0.4$ , (b)  $D/J = -0.1$ , (c)  $D/J = -0.2$ , (d)  $D/J = -0.6$ .

Firstly, we take the number of the spin  $N$  to be an odd number. Because of the antiferromagnetic coupling, all the spin bonds cannot reach the minimum energy at the same time, system exhibits geometric frustration phenomenon and the behavior of



magnetic susceptibility will be more interesting. In Figs. 2 and 3 they show the temperature dependence of the magnetic susceptibility multiplied by temperature  $\chi T$  for the spin quantum numbers of impurity being 1 and  $3/2$  respectively and  $N = 21$ . Under the different anisotropy of impurity and different host-impurity exchange interaction, it is found that the  $\chi T$  increases almost linearly with temperature in the higher temperature, which is consistent with the result of open chain, but it is significantly different with that of the open chain in the low temperature [5]. The  $\chi T$  shows three obvious variation behaviors with temperature decreasing. In the first case, the  $\chi T$  rapidly increases and tends to a finite value as temperature approaches to zero. In the second case, the  $\chi T$  tends to a finite value almost horizontally with the temperature decreasing, which is consistent with the result of Delta chain [2]. In the third case, the  $\chi T$  decreases rapidly and tends to a finite value with the temperature closing zero. In addition, we find that the value of  $\chi T$  in zero temperature limit is related to the value of impurity anisotropy and host-impurity exchange interaction. Comparing Fig. 2 and Fig. 3 we also find that the values of  $\chi T$  in zero temperature limit are different for spin quantum numbers of the impurity taking 1 and  $3/2$ , indicating that the limit value of  $\chi T$  is related to the spin quantum number of the impurity, which is consistent with the open chain.

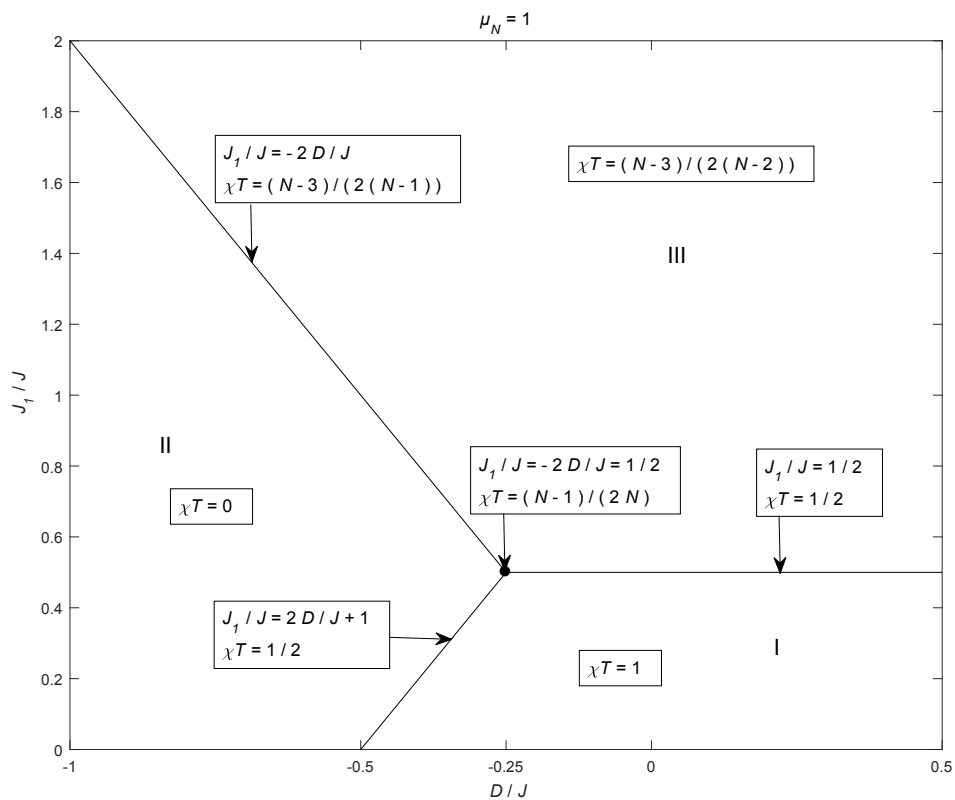


Fig.4. The value of  $\chi T$  in the parameter space of strength  $D$  of anisotropy of impurity and host-impurity exchange interaction  $J_1$  as  $T \rightarrow 0$ .  $\mu_N = 1$ .

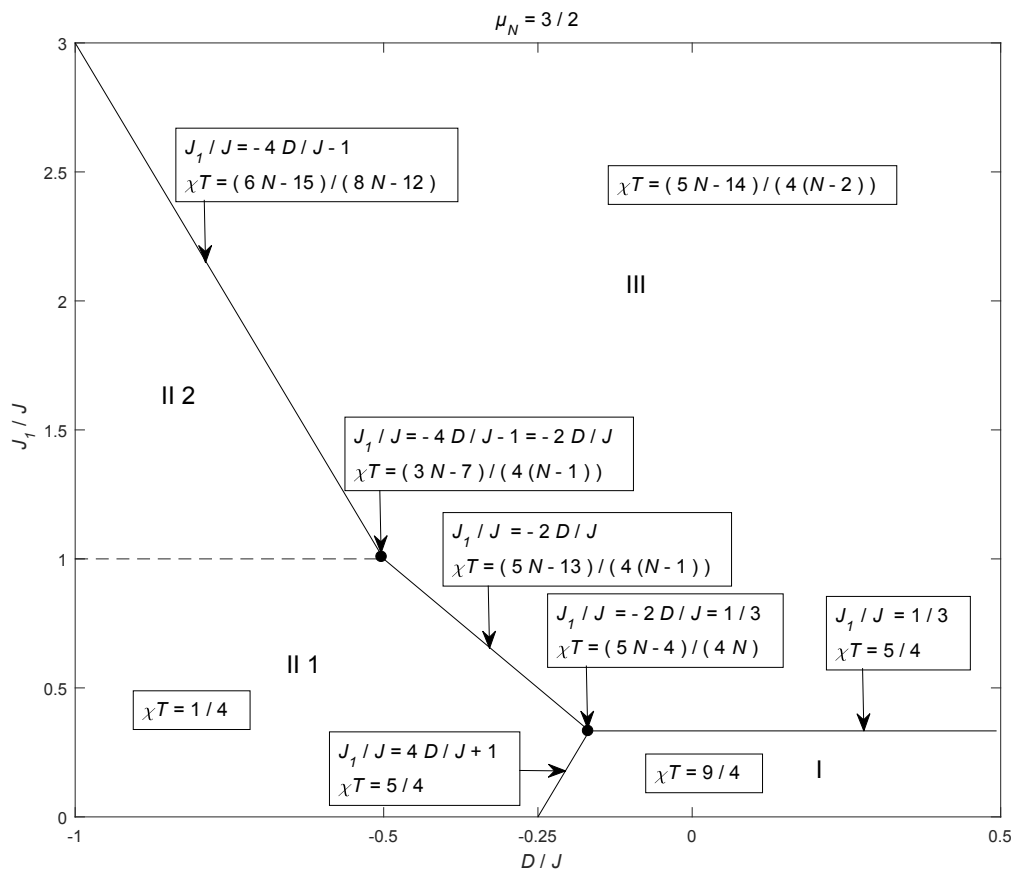


Fig.5. The value of  $\chi T$  in the parameter space of strength  $D$  of anisotropy of impurity and host-impurity exchange interaction  $J_1$  as  $T \rightarrow 0$ .  $\mu_N = 3/2$ .

Because the system has no long-range magnetic order in the finite temperature, the transition temperature is zero. According to Curie's law,  $\chi T = C$ , in zero temperature limit the values of  $\chi T$  for various anisotropy of impurity and host-impurity exchange interaction are different, indicating that the Curie constant associates with the anisotropy of impurity and host-impurity exchange interaction. In order to determine the Curie constant of the system, we take the zero temperature limit of formula (23) to obtain the Curie constants of the system for different parameters. The specific results are shown in Fig. 4 and Fig. 5. It can be seen that for the impurity with spin quantum number 1 and 3/2, although the values of Curie

constant are different, the values are all distributed in three regions, the boundary line and intersection points of the regions. In three regions, the value of the  $\chi T$  in zero temperature limit can be expressed as,

$$\lim_{T \rightarrow 0} \chi T = \begin{cases} (\mu_N)^2, & \text{phase I} \\ (\mu_N^Z)_{min}^2, & \text{phase II} \\ \frac{(\mu_N)^2 + (\mu_N^Z)_{min}^2}{2}, & \text{the boundary of phase I and phase II} \\ \frac{(2(\mu_N)^2 + 1)(N - 2) + 2\mu_N(1 - N) + 1}{2(N - 2)}, & \text{phase III} \\ (\mu_N)^2 - \mu_N + \frac{1}{2}, & \text{the boundary of phase I and phase III} \end{cases} \quad (25)$$

It is found that the Curie constant in each region is independent of the value of the anisotropy of the impurity and the host-impurity exchange interaction, and is related to the spin quantum number of impurity. In particular, in the phase III, the Curie constant is also related to the total number of spin.

To clarify this issue, we determine the ground state of the system in each region. Using the up and down arrows to represent the directions of the host spin and the number  $+1, 0, -1$  and  $+\frac{3}{2}, +\frac{1}{2}, -\frac{1}{2}, -\frac{3}{2}$  represent the spin states of the impurity with spin quantum number of 1 and 3/2 respectively, the ground state of the system can be expressed as follows,

For  $\mu_N = 1$ ,

$$\text{ground state} = \begin{cases} |\dots \uparrow \downarrow \uparrow - 1 \downarrow \uparrow \downarrow \dots\rangle, & \text{phase I} \\ |\dots \uparrow \downarrow \uparrow 0 \downarrow \uparrow \downarrow \dots\rangle, & \text{phase II} \\ |\dots \uparrow \downarrow \uparrow - 1 \uparrow \downarrow \uparrow \dots \uparrow \uparrow \dots\rangle, |\dots \uparrow \downarrow \uparrow - 1 \uparrow \downarrow \uparrow \dots \downarrow \downarrow \dots\rangle & \text{phase III} \end{cases} \quad (26)$$

due to the upper and lower symmetry of Ising spin, the antisymmetric state is also the ground state of the system.

For  $\mu_N = 3/2$ ,

$$\text{ground state} = \left\{ \begin{array}{l} |\dots\uparrow\downarrow\uparrow - \frac{3}{2}\downarrow\uparrow\downarrow\dots\rangle, \text{ phase I} \\ |\dots\uparrow\downarrow\uparrow - \frac{1}{2}\downarrow\uparrow\downarrow\dots\rangle, \text{ phase II1} \\ |\dots\downarrow\uparrow\downarrow - \frac{1}{2}\uparrow\downarrow\uparrow\dots\rangle, |\dots\uparrow\downarrow\uparrow - \frac{1}{2}\uparrow\downarrow\uparrow\dots\rangle \\ |\dots\uparrow\downarrow\uparrow - \frac{1}{2}\downarrow\uparrow\downarrow\dots\rangle, |\dots\uparrow\downarrow\uparrow - \frac{1}{2}\uparrow\downarrow\uparrow\dots\rangle \\ \text{, phase II2} \\ |\dots\uparrow\downarrow\uparrow - \frac{3}{2}\downarrow\uparrow\downarrow\dots\rangle \text{ and } |\dots\uparrow\downarrow\uparrow - \frac{3}{2}\uparrow\downarrow\uparrow\dots\rangle \\ \text{, phase III} \end{array} \right. \quad (27)$$

the ground state of the system also includes the antisymmetric state.

Here, the Curie constant of phase II1 and phase II2 in the system of  $\mu_N = 3/2$  are equivalent, so we separate them with a dashed line in Fig. 5.

In phase I, due to the weak host-impurity exchange interaction, the impurity spin and connected spin shows ferromagnetic arrangement, and the magnetic susceptibility of the system shows ferromagnetic temperature behavior similar to that of an open chain, and the Curie constant equals to the square of the net spin [5]. In phase II1, the frustration of the exchange interaction and the easy-plane anisotropy of the impurity are superposed in the same direction to minimize the value of spin of the impurity, and the ground state of the system is in nondegenerate. In phase II2, for  $\mu_N = 3/2$ , the value of the spin state of impurity is same to that of the host spin, so the ground state of the system is degenerate. In region III, when the anisotropy of the impurity is positive, the large host-impurity exchange interaction and anisotropy demand the spin of impurity taking the maximum value to ensure the anti-parallel arrangement of the spin of the impurity and the neighboring spin of the host. When the anisotropy of the impurity is negative, the larger host-impurity exchange interaction is dominant in the competition with the anisotropy of the impurity, which also leads to the impurity

taking the maximum spin value and the anti-parallel arrangement of the spin of the impurity and the neighboring spin of the host. In this case, the frustration leads to the spins in the ring cannot get simultaneously the minimum energy, and the spin pair with same direction can appear at any position in the ring, indicating that the ground state of system is degenerate, which may be the reason that the magnetic susceptibility multiplied by temperature  $\chi T$  is related to the total number of spin  $N$ . At the boundary line between phase I and phase II, the magnetic susceptibility multiplied by temperature  $\chi T$  equals to the average value of the values in the two phases.

Since the Curie constant is related to the spin configuration of system at ground state, we can discuss the ground state entropy of system. Using equation (5) and the transfer matrix calculation, we find the ground state entropy of the system can be expressed as,

For  $\mu_N = 1$ ,

$$S = \begin{cases} \ln(2), & \text{phase I and phase II} \\ \ln(2(N-2)), & \text{phase III} \\ \ln(4), & \text{the boundary of phase I and phase II} \\ \ln(2(N-1)), & \text{the boundary of phase I and phase III} \\ \ln(2N), & \text{the intersection of phase I, phase II and phase III} \end{cases} \quad (28)$$

For  $\mu_N = 3/2$ ,

$$S = \begin{cases} \ln(2), & \text{phase I and phase II1} \\ \ln(2(N-1)), & \text{phase II2} \\ \ln(2(N-2)), & \text{phase III} \\ \ln(4), & \text{the boundary of phase I and phase II1} \\ \ln(2(N-1)), & \text{the boundary of phase I and phase III} \\ \ln(2(2N-3)), & \text{the boundary of phase II2 and phase III} \\ \ln(2N), & \text{the intersection of phase I, phase II1 and phase III} \\ \ln(4(N-1)), & \text{the intersection of phase II1, phase II2 and phase III} \end{cases} \quad (29)$$

In phases I and phase II, for  $\mu_N = 1$  and phases I and II1, the ground state entropy is  $\ln(2)$ , indicating the system is in the upper and lower symmetric state. In

phase II2, for  $\mu_N = 3/2$ , the number of state is 2 more than that in phase III because of the impurity spin being in  $1/2$  state and the ground state entropy is  $\ln(2(N-1))$ . And on the boundary line between the two phases, the ground state entropy equals the natural logarithm of the sum of all the ground states in the two phases. In the intersection of phases, the ground state entropy equals the natural logarithm of the sum of all the ground states in the neighboring phases.

When the number  $N$  of spin of the ring is even, the system does not have the frustrated phenomenon, but the system may also shows the ferromagnetic characteristics, and the magnetic susceptibility shows similar behaviors to those in Fig. 2 and Fig. 3. Compared with the number of spin  $N$  being odd, in zero temperature limit the Curie constant is also determined by the ground state of the system, namely, by the anisotropy of impurity and the host-impurity exchange interaction. Since there is no frustrated effect and degeneracy in the ground state of the system, the magnetic susceptibility multiplied by temperature  $\chi T$  in zero temperature limit is equal to the square of the net spin in each phase, independent of the number of spin,  $N$ , which is consistent with the conclusion about the open chain [5].

In  $\mu_N = 1$  system, the ground state can be divided into two regions,

$$\text{ground state} = \begin{cases} |\cdots\uparrow\downarrow - 1\uparrow\downarrow\cdots\rangle, & \frac{J_1}{J} + \frac{2D}{J} > -1 \\ |\cdots\uparrow\downarrow 0\uparrow\downarrow\cdots\rangle, & \frac{J_1}{J} + \frac{2D}{J} < -1 \end{cases} \quad (30)$$

where due to the upper and lower symmetry of Ising spin, the antisymmetric state is also the ground state of the system.

Since the absolute value of the net spin in both phases is  $1/2$ , the Curie constant

of the system is  $1/4$  in both phases and at boundary between the two phases.

In  $\mu_N = 3/2$  system, the ground state can also be divided into two regions,

$$\text{ground state} = \begin{cases} \left| \dots \uparrow \downarrow \uparrow - \frac{3}{2} \uparrow \downarrow \uparrow \dots \right\rangle, \frac{J_1}{J} + \frac{4D}{J} > -1 \\ \left| \dots \uparrow \downarrow \uparrow - \frac{1}{2} \uparrow \downarrow \uparrow \dots \right\rangle, \frac{J_1}{J} + \frac{4D}{J} < -1 \end{cases} \quad (31)$$

the ground state of the system also includes the antisymmetric state.

Since the absolute value of the net spin is 1 and 0 in the two phases, the Curie constant of the system is 1 and 0 in the two phases, respectively, and it is  $1/2$  on the boundary line between the two phases.

For  $\mu_N = 1$  and  $\mu_N = 3/2$ , the ground state entropy is  $\ln(2)$  in the two phases, and it is  $\ln(4)$  on the boundary line between the two phases.

#### 4 . Conclusion

Although the finite antiferromagnetic Ising closed ring doped with spin-1 and  $-3/2$  impurities has no spontaneous magnetization at finite temperature, it shows ferromagnetic characteristics at low temperature. Due to the anisotropy of the impurity and host-impurity exchange interaction, its magnetic susceptibility multiplied by temperature  $\chi T$  presents three types of behavior with temperature decreasing in the low temperature, bending upward, horizontally and downward tends to a finite value at zero temperature. In the parameter space of the anisotropy of the impurity and host-impurity exchange interaction, when the number of spin is even, the ground state of the system has two nondegenerate phases. When the number of spin is odd, the system is frustrated, and there are nondegenerate phases and degenerate



phases in the ground state. In the nondegenerate phase, the Curie constant is equal to the square of the net spin of the system and the ground state entropy is  $\ln(2)$ , and on the boundary line of two nondegenerate phases, the Curie constant is equal to the average value of the values in the two neighboring phases and the ground state entropy is  $\ln(4)$ . In the degenerate phase, the Curie constant and ground state entropy are dependent on the number of spin in the ring, except for the Curie constant being a constant in degenerate state II2 for  $\mu_N = 3/2$ . According to the results of this paper, we speculate that for any finite Ising antiferromagnetic system, when the ground state is nondegenerate, the magnetic susceptibility multiplied by temperature  $\chi T$  in the zero temperature limit equals the square of the net spin, and when the ground state is degenerate, it is related to the number of spins in the system. In high temperature limit, the  $\chi T$  is related to not only the number of spin but also spin quantum number of impurity.

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