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**THERMODYNAMICS OF THE DILUTED SPIN HEISENBERG
CHAIN WITH SINGLE ION ANISOTROPY**

by

Salmah Ahmed

**A Thesis
Submitted to the
Faculty of The Graduate College
in partial fulfillment of the
requirements for the
Degree of Master of Arts
Department of Physics**

**Western Michigan University
Kalamazoo, Michigan
December 1987**

**THERMODYNAMICS OF THE DILUTED SPIN HEISENBERG
CHAIN WITH SINGLE ION ANISOTROPY**

Salmah Ahmed, M.A

Western Michigan University, 1987

The thermodynamics of the one-dimensional diluted Heisenberg magnet of classical spins in the presence of single ion anisotropy is calculated. The magnetization, susceptibility, energy and specific heat are determined as functions of the magnetic concentration and single ion anisotropy for both ferromagnetic and antiferromagnetic couplings. Spin-spin correlation functions and the elastic scattering are also calculated for various values of anisotropy and spin concentration for the ferromagnetic system.

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Salmah Ahmed

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CHAPTER I

INTRODUCTION

The work done in this thesis solved exactly for the thermodynamics of spin chain in the presence of single ion anisotropy, specifically for the chains which are mixtures of magnetic and non-magnetic ions. These systems are found to be good representation of compounds formed from CsNiF_3 and CsMnF_3 . This solution can be done on the computer by essentially exact techniques involving the sum over chain fragments.

The physics of systems with less than three dimensions, such as the one solved here, has been widely studied in recent years, especially since the discovery of real materials whose properties closely approximate those of one- or two-dimensional lattice models. The reason to study the system in one dimension is largely because it is easy to construct models which in some cases can be solved exactly. The classical models studied in this thesis as opposed to quantum mechanical models are widely being used in studying such systems because many of the properties of experimental systems at not too low temperatures are successfully treated by such models, and also classical models are usually more solvable for exact solutions compared to the method of quantum mechanics. There are numbers of solutions which exist in one- and two-dimensional systems for models based on classical spins such as the one

studied in this thesis. Examples in one dimension are (1) The Ising, (2) The Classical Spin Heisenberg, (3) The X-Y models and many solutions of the continuum model. For two-dimensional systems there exist a variety of solutions of Ising and vertex system.

Thermodynamic properties in lower dimensional magnetic spin systems have long been studied theoretically as well as experimentally. In the study of one-dimensional magnetic materials, the model which has found considerable success in describing experimental system is the classical spin Heisenberg model. For isotropic exchange coupling in zero applied field, Fisher¹ provided an exact solution for the thermodynamic behavior and the static spin correlation function. On the other hand, Joyce² has solved the problems for anisotropic exchange interactions using the same model. This model has been used to fit the experimentally determined magnetic properties of many chain compounds and has given good representations of such properties as the spin-spin correlation lengths, magnetic susceptibilities, and specific heats over a wide range of temperature for both ferromagnetic and antiferromagnetic systems.

The Heisenberg model is not only useful in studying the properties of pure infinite chain compounds, but it can be used also for the diluted or alloyed magnetic materials like this case with zero applied field. In diluted materials, the system consists of random mixtures of spins with non-magnetic impurities, while in alloys the spins mix with spins of differing magnitudes and inter-spin exchange coupling. Examples of experimental works on diluted chain compounds which are related to classical model solutions are

$(\text{CD}_3)_4\text{NMn}_x\text{Cu}_{1-x}\text{Cl}_3$, worked by Endoh et al.³ and $\text{CsMn}_{1-x}\text{Br}_3$ by Furrer and Gudel.⁴ Theoretical solutions for a diluted system in the absence of external field achieved very good agreement with experimental data in those two types of materials.^{3,4} In both of the above experimental efforts, the classical spin Heisenberg model was used to fit the experimental data.

These diluted and alloyed classical magnetic systems have not been previously solved for the single ion anisotropy terms which often occur in one-dimensional chain compound. The result presented in this thesis will hopefully stimulate experiments on such systems so as to determine the validity of the classical spin description for this kind of system.

The work reported here is concerned with the thermodynamics and static correlation behavior in the diluted one-dimensional classical Heisenberg model in the presence of single ion anisotropy. The magnetization, susceptibility, energy, and specific heat of the diluted system are calculated as functions of magnetic concentration and single ion anisotropy. Following the procedures in Dong and McGurn,⁵ the properties for the finite chains were first determined in order to obtain the properties of the diluted system. Then the weighted sum of such terms is found where the weight multiplying a given term in the sum over the finite chain properties is the probability that a chain for that particular length occurs in the diluted system. Taking the sums on chains of up to forty spins in length for magnetic concentrations of $p = 0.8$ and 0.5 give very accurate values to the properties of this system where for the pure

system p = 1.0.

CHAPTER II

DILUTED CLASSICAL SPIN HEISENBERG CHAIN

Theory

For a case in three-dimensional crystal where the magnetic ions have a strong coupling in one direction and very weak in the other two, the system can be discussed as a one-dimensional system. In this "one-dimensional" system, the Hamiltonian can be written as

$$H = -J \sum_i \vec{S}_i \cdot \vec{S}_{i+1} + \sum_i V(\vec{S}_i) \quad (2.1)$$

Here $V(\vec{S}_i)$ is the interaction potential between magnetic ions and the orbital moment of the crystal field in the presence of magnetic dipoles. J is a nearest-neighbour exchange coupling and $\{\vec{S}_i\}$ are classical unit vectors at the discrete sites of the lattice.

Because of the strong crystal field and the very weak dipole forces, the moment of the system is often quenched. Therefore, the first approximation can be taken and equation (2.1) becomes

$$H = -J \sum_i \vec{S}_i \cdot \vec{S}_{i+1} \quad (2.2)$$

A spin one ion like Ni^{2+} usually has good orbital quenching where the most general form of its interaction potential is

$$V(\vec{S}_i) = A(S_i^Z)^2 + \text{constant}$$

Hence, the total Hamiltonian is

$$H = -J \sum_i c_i c_{i+1} S_i \cdot S_{i+1} - D \sum_i c_i (S_i^Z)^2 \quad (2.3)$$

where D is the strength of the single site anisotropy and $C_i = 1$ or 0 depending on whether or not a spin is present on the i^{th} site. The system is ferromagnetic if $J > 0$ and antiferromagnetic if $J < 0$.

For the system of non-magnetic impurities (i.e. $C_k = 0$ for certain k in equation (2.3)), the infinite chain tends to break up into isolated chain segments of finite length. Assuming the non-magnetic impurities occur at random, and there is no correlation between them, then the partition function of the above Hamiltonian can be written as a product of the individual chain as

$$Z(T, D, p) = \prod_{L=1}^{\infty} [Z_L(T, D)]^{N(1-p)^2 p^L} \quad (2.4)$$

Here p is the concentration of spins present in the system $N \rightarrow \infty$ lattice site and $Z_L(T, D)$ is the partition function for a chain of L spins. Then the magnetization, energy, specific heat and magnetic susceptibility per lattice site of the diluted system can be written following the notation in Dong and McGurn⁵ as

$$M(T, D, p) = (1 - p)^2 \sum_{L=1}^{\infty} p^L M_L(T, D) \quad (2.5)$$

$$E(T, D, p) = (1 - p)^2 \sum_{L=1}^{\infty} p^L E_L(T, D) \quad (2.6)$$

$$C(T, D, p) = (1 - p)^2 \sum_{L=1}^{\infty} p^L C_L(T, D) \quad (2.7)$$

and

$$X(T, D, p) = (1 - p)^2 \sum_{L=1}^{\infty} p^L X_L(T, D) \quad (2.8)$$

where $M_L(T,D)$, $E_L(T,D)$, $C_L(T,D)$ and $X_L(T,D)$ are the magnetic moment, total energy, specific heat and magnetic susceptibility of a chain of L spins.

Again, considering only for chain of L spins, the Hamiltonian of equation (2.2) can be written as

$$H_L = -J \sum_{i=1}^{L-1} S_i \cdot S_{i+1} - \frac{D}{2} \sum_{i=1}^{L-1} [(S_i^Z)^2 + (S_{i+1}^Z)^2] - \frac{D}{2} (S_L^Z)^2 - \frac{D}{2} (S_1^Z)^2 \quad (2.9)$$

The thermodynamics properties of this equation have to be solved in order to obtain $M_L(T,D)$, $E_L(T,D)$, $C_L(T,D)$ and $X_L(T,D)$. The partition function $Z(T,D)$ of equation (2.4) can be written following the notation in Blume et al.⁶ as

$$Z_L(T,D) = \int \dots \int dS_1 \dots dS_L \exp \left\{ \frac{\beta D}{2} [(S_1^Z)^2 + (S_L^Z)^2] \right\} \times \prod_{i=1}^{L-1} \exp[V(\hat{S}_i, \hat{S}_{i+1})] \quad (2.10)$$

where

$$V(\hat{S}_i, \hat{S}_{i+1}) = -J \hat{S}_i \cdot \hat{S}_{i+1} - \frac{D}{2} ((S_i^Z)^2 + (S_{i+1}^Z)^2) \quad (2.11)$$

and $\beta = J/kT$. $dS_i = \sin \theta_i d\theta_i d\phi_i$ where θ_i and ϕ_i are the polar and azimuthal angles of the i^{th} spin and this term represents an element of solid angle for that i^{th} spin.

Equation (2.10) can be written in terms of the eigenvalues and eigenvectors of the eigenvalue problem defined by the integral equation

$$\int \exp[\beta V(\vec{S}_1, \vec{S}_2)] \psi_n(\vec{S}_2) d\vec{S}_2 = \lambda_n \psi_n(\vec{S}_1) \quad (2.12)$$

where $n = 0, 1, 2, \dots$ are the labels of the eigenstates.

Hence

$$\exp[\beta V(\vec{S}_1, \vec{S}_{1+1})] = \sum_{n=0}^{\infty} \lambda_n \psi_n^*(\vec{S}_1) \psi_n(\vec{S}_{1+1}) \quad (2.13)$$

Then equation (2.9) becomes

$$Z_L(T, D) = \sum_n \left| \int ds e^{\beta D(S^z)^2/2} \psi_n(s) \right|^2 \lambda_n^{L-1} \quad (2.14)$$

From Blume et al.,⁶ the internal energy for L spins is given by

$$E_L = -J \sum_i \langle \vec{S}_i \cdot \vec{S}_{i+1} \rangle - D \sum_i \langle (S_i^z)^2 \rangle \quad (2.15)$$

Then the specific heat is calculated by simply taking the derivative of the energy equation with respect to temperature.

$$C_L(T, D) = \frac{\partial}{\partial T} E_L(T, D) \quad (2.16)$$

The magnetization and magnetic susceptibility of the L spins chain are given by the standard relation

$$M_L(T, D) = \frac{\partial}{\partial H} \ln Z_L(T, D) \quad (2.17)$$

$$\chi_L(T, D) = \frac{\partial}{\partial H} M_L(T, D) \quad (2.18)$$

To obtain results from equations (2.6) to (2.8) for energy, specific heat and magnetic susceptibility, the eigenvalue problem defined in equation (2.12) and all the equations from (2.15) to (2.18) need to be evaluated numerically. This procedure will be discussed in the next section.

Since the work discussed in this thesis deals with the system in the absence of an external magnetic field, it is known that the magnetization does not exist. Therefore, in order to calculate the magnetic susceptibility, an assumption has to be made that the

applied field is not zero and then solve the equation in the limit that $H = 0$. In the presence of an external field, the Hamiltonian of chain of L spins is

$$H_L = -J \sum_i \vec{S}_i \cdot \vec{S}_{i+1} - \mu g H \sum_i S_i^Z - D \sum_i (S_i^Z)^2 \quad (2.19)$$

The partition function is then

$$Z_L = \int e^{-\beta H_L} d\vec{S}_i \quad (2.20)$$

Evaluating the magnetization and magnetic susceptibility defined in equations (2.17) and (2.18) at $H = 0$ yields

$$M_L(T, D) \Big|_{H=0} = \frac{\partial}{\partial \beta H} \ln Z_L(T, D) \Big|_{H=0}$$

and

$$\chi_L(T, D) \Big|_{H=0} = \frac{\partial}{\partial H} M(T, D, H) \Big|_{H=0}$$

The equation of magnetic susceptibility above can be expressed also in terms of the correlation function as

$$\chi = (\beta \mu^2 g^2)^{-1} \sum_{j=1}^L \overline{\langle S_i^Z \cdot S_j^Z \rangle} \quad (2.21)$$

where $\overline{\langle S_i^Z \cdot S_j^Z \rangle}$ is the average correlation function.

The static properties of this 'one-dimensional' system which is defined by equation (2.2) can be used to calculate the cross section for neutron scattering $S(\vec{q})$ in the quasielastic approximation. This system with only one kind of atom was first solved by Fisher¹ and the solution utilizes the expansion

$$e^{\beta H_{1,2}} = e^{\beta J \vec{S}_1 \cdot \vec{S}_2} = 4\pi \sum_{\lambda, m} \lambda_{\lambda}(\beta J) Y_{\lambda m}(\vec{S}_1) Y_{\lambda m}^*(\vec{S}_2) \quad (2.22)$$

Here

$$\lambda_l(\beta J) = (1/2) \int_{-1}^{+1} e^{\beta J x} P_l(x) dx \quad (2.23)$$

where $Y_{lm}(\vec{S}_i)$ are spherical harmonics and $P_l(x)$ are Legendre Polynomials. Evaluating equation (2.23) yields

$$\lambda_0(\beta J) = (\sinh \beta J) / \beta J \quad (2.24)$$

From Thorpe⁷ the cross-section for neutron scattering is given by the wave vector dependent susceptibility

$$S(\vec{q}) = (1/N) \sum_{i,r} e^{i \cdot \vec{q} \cdot \vec{r}} \langle \vec{S}_i \cdot \vec{S}_{i+r} \rangle \quad (2.25)$$

Following the notation in that paper,⁷ equation (2.25) can be rewritten as

$$S(q) = (1/N) \sum_{i,r} e^{i q a r} \langle \vec{S}_i \cdot \vec{S}_{i+r} \rangle \quad (2.26)$$

This expression depends only on the component of $\vec{q}$ (wave vector of neutron) chain which is denoted by q and a is the interatomic spacing. Considering only the z -direction so that only $l = 1$, $m = 0$ term contributes and

$$\langle S_i^z \cdot S_{i+r}^z \rangle = (1/3) \left(\frac{\lambda_1}{\lambda_0} \right)^r \quad (2.27)$$

equation (2.26) becomes

$$S(q) = (1/N) \sum_{i,r} e^{i q a r} \left(\frac{\lambda_1}{\lambda_0} \right)^{|r|} \quad (2.28)$$

where the summation over r goes over all positives and negatives integers. Letting $u = \lambda_1/\lambda_0$ and evaluating equation (2.23) leads to

$$u = \lambda_1 / \lambda_0 = \coth(\beta J) - 1/(\beta J) \quad (2.29)$$

For the diluted system when $D = 0$ and $q = 0$, the sum defined by equation (2.26) can be written as

$$\begin{aligned} S(q) &= \frac{1}{3}(1-p)^2 \sum_{L=1}^{\infty} \sum_{i=1}^L \sum_{j=1}^L u^{|j-i|} p^L \\ &= p(1+up)/3(1-up) \end{aligned} \quad (2.30)$$

where u is defined as in equation (2.29) and $j = i + r$. This sum is just equal to the magnetic susceptibility for isotropic chain system. However, when $q \neq 0$ the sum over the exponential term of equation (2.28) will contribute a cosine function and the cross-section for the neutron scattering from the diluted system can be rewritten as

$$S(q) = p[1 - (up)^2] / 3[1 + (up)^2 - 2up \cos(qa)]. \quad (2.31)$$

Both of these results are extended to include the $D \neq 0$ case which is obtained from equation (2.26) calculated in the basis of states from equation (2.12).

CHAPTER III

RESULTS AND COMPARISONS

To solve for the partition function for L spins, the eigenvalue problem defined by equation (2.12) can be rewritten into the form of a matrix eigenvalue problem. Letting $\Psi_n(S) = \Psi_{lm}(x) e^{im\phi} / 2\pi$ where $x = \cos\theta$ and inserting this into equation (2.12) gives the following eigenvalue equation

$$2\pi \int dx' \exp \left\{ \beta J x x' + \frac{\beta D}{2} (x + x') \right\} I_m(\beta J[(1-x^2)(1-x'^2)]^{1/2}) \Psi_{lm}(x') = \lambda_{lm} \Psi_{lm}(x) \quad (3.1)$$

where

$$I_m(x) = \frac{1}{2\pi} \int_0^{2\pi} \exp(x \cos \phi - im\phi) d\phi = I_m(-x) \quad (3.2)$$

Then, equation (3.2) can be written as a matrix equation by the use of Gaussian integration formula

$$\int_{-1}^{+1} f(x) dx = \sum_{j=1}^N w_j f(x_j) \quad (3.3)$$

where $N \rightarrow \infty$ and the weight w_j and points x_j are given in tables. The matrix eigenvalues equation becomes

$$\sum_{j=1}^N w_j G_m(x_1, x_j) \Psi_{lm}(x_j) = \lambda_{lm} \Psi_{lm}(x_1) \quad (3.4)$$

where

$$G_m(x, x') = 2\pi \exp[\beta J x x' + \frac{\beta D}{2} (x + x')] I_m(\beta J[1-x^2)(1-x'^2)]^{1/2} \quad (3.5)$$

letting

$$H_{1j}^{(m)} = \sqrt{w_1} G_m(x_1, x_j) \sqrt{w_j} \text{ and } \phi_i^{(lm)} = \sqrt{w_1} \Psi_{lm}(x_1)$$

and substituting these into equation (3.5) yields

$$\sum_{j=1}^N H_{1j}^{(m)} \phi_j^{(lm)} = \lambda_{lm} \phi_i^{(lm)} \quad (3.6)$$

Since these calculations concern only the chain of finite length, only the $m = 0$ solution of equation (3.6) exist. The partition function of equation (2.14) can be written in terms of the solution of equation (3.6) as

$$Z_L(T, D) = \sum_{\lambda=0}^{\infty} |a_{\lambda}|^2 \lambda_{\lambda_0}^{L-1} \quad (3.7)$$

where

$$a_{\lambda} = \sqrt{2\pi} \sum_{j=1}^{\infty} \sqrt{w_1} \exp(\beta D x_j / 2) \phi_i^{(lm)} \quad (3.8)$$

Values for $E_L(T, D)$ and $C_L(T, D)$ are then obtained from equations (2.15) and (2.16) by numerically calculating the derivatives of $Z_L(T, D)$ and $E_L(T, D)$ with respect to β and T . Once these properties are calculated for chains of length L , the sums in equations (2.5) to equation (2.8) can be used to evaluate the properties of the diluted systems. Then the susceptibility of the diluted system is obtained by numerically differentiating $M_L(T, D)$ with respect to H as mentioned in the previous section. Finally, to obtain the neutron scattering, equation (2.25) needs to be evaluated numerically.

In Figures 1a through 1d the graphs of energy per spin versus temperature for magnetic concentrations $p = 0.8$ and 0.5 are presented for the ferromagnetic system. The curves for different ratio D/J are plotted on the same graph. The correct high and low temperature limits are obtained and the comparison of the curves for

negative anisotropy can be made by referring to the paper by Dong and McGurn.⁵ In all the figures, the curves presented are found to closely approach the high temperature limit (i.e. $-(D/J)p/3$) at the right hand edge of the drawings.

The graphs of specific heat versus temperature are shown in Figures 2a through 2d for both magnetic concentrations $p = 0.8$ and 0.5 and with different values of anisotropy. Again the correct high temperature limit are observed which closely equal to $p^{2/3} + 4p(D/J)^{2/45}$. Table 1 presents the results for energy and specific heat obtained from the high temperature limit and also from the computer calculation. In both cases (i.e. energy and specific heat), it is found that all characteristics of the curves in the ferromagnetic coupling are exactly the same for the same magnitude but opposite sign of anisotropy and the same magnetic concentration in the antiferromagnetic coupling. This fact can be seen from equation (2.9) where for the antiferromagnetic system $-J$ is used instead of $+J$ but the summation is still the same.

The magnetic susceptibilities for the ferromagnetic and the antiferromagnetic system are presented in Figures 3 and 4 respectively. From Table II to V, the results obtained from the low and high temperature limits and from the computer calculations are shown for both ferromagnetic and antiferromagnetic couplings. The figures show that the isotropic susceptibility seems to separate the susceptibility for negative and positive anisotropy. However, at low temperature in the ferromagnetic case, the values of susceptibility in the z-direction for positive anisotropy are getting

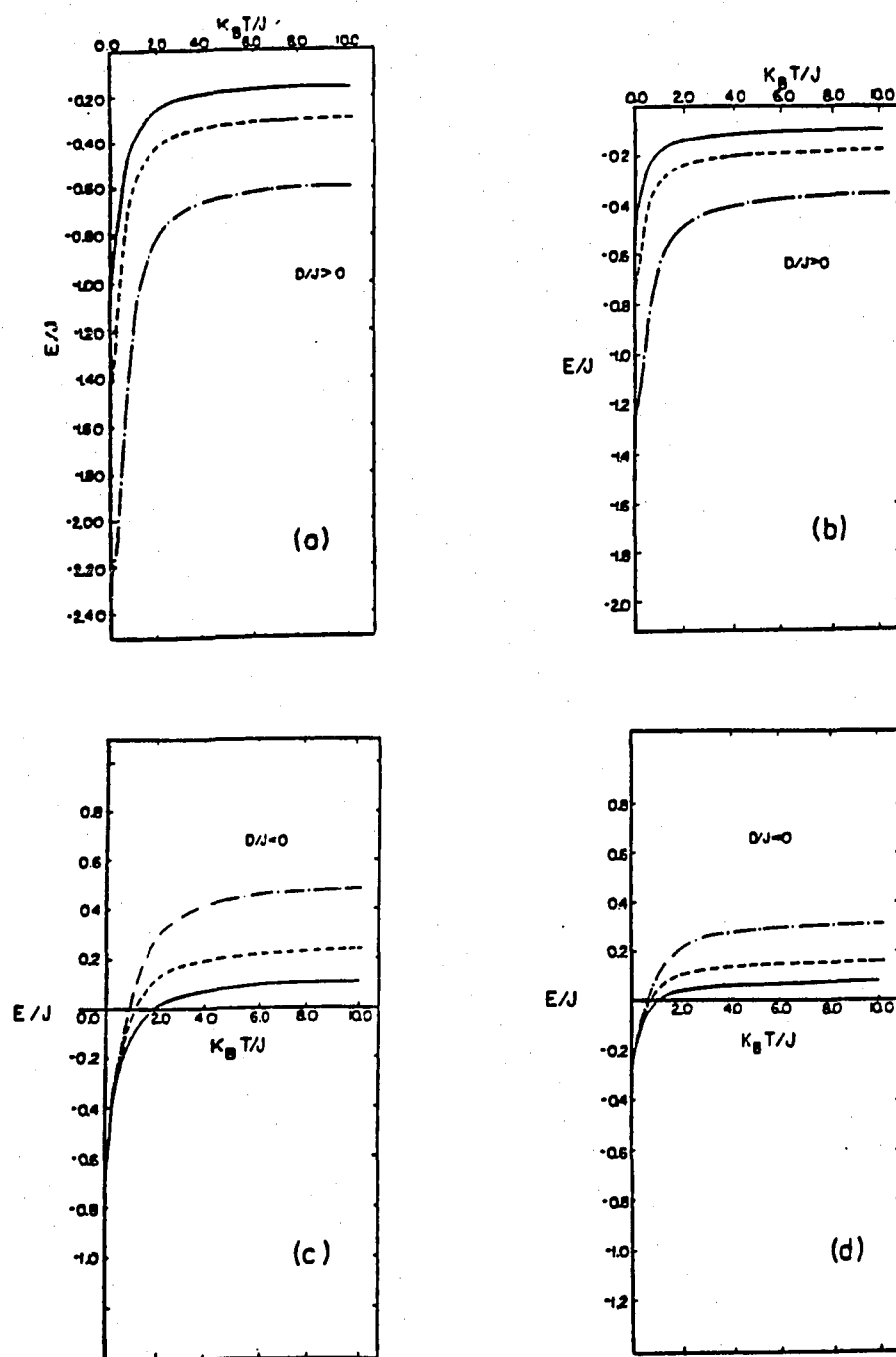


Figure 1. Ferromagnetic energy per lattice site versus $k_B T/J$ for $D/J = 2.0$ (dot-dashed), 1.0 (dashed) and 0.5 (solid) for (a) $p = 0.8$, (b) $p = 0.5$. Curves for $D/J = -2.0$ (dot-dashed), -1.0 (dashed) and -0.5 (solid) for (c) $p = 0.8$ and (d) $p = 0.5$.

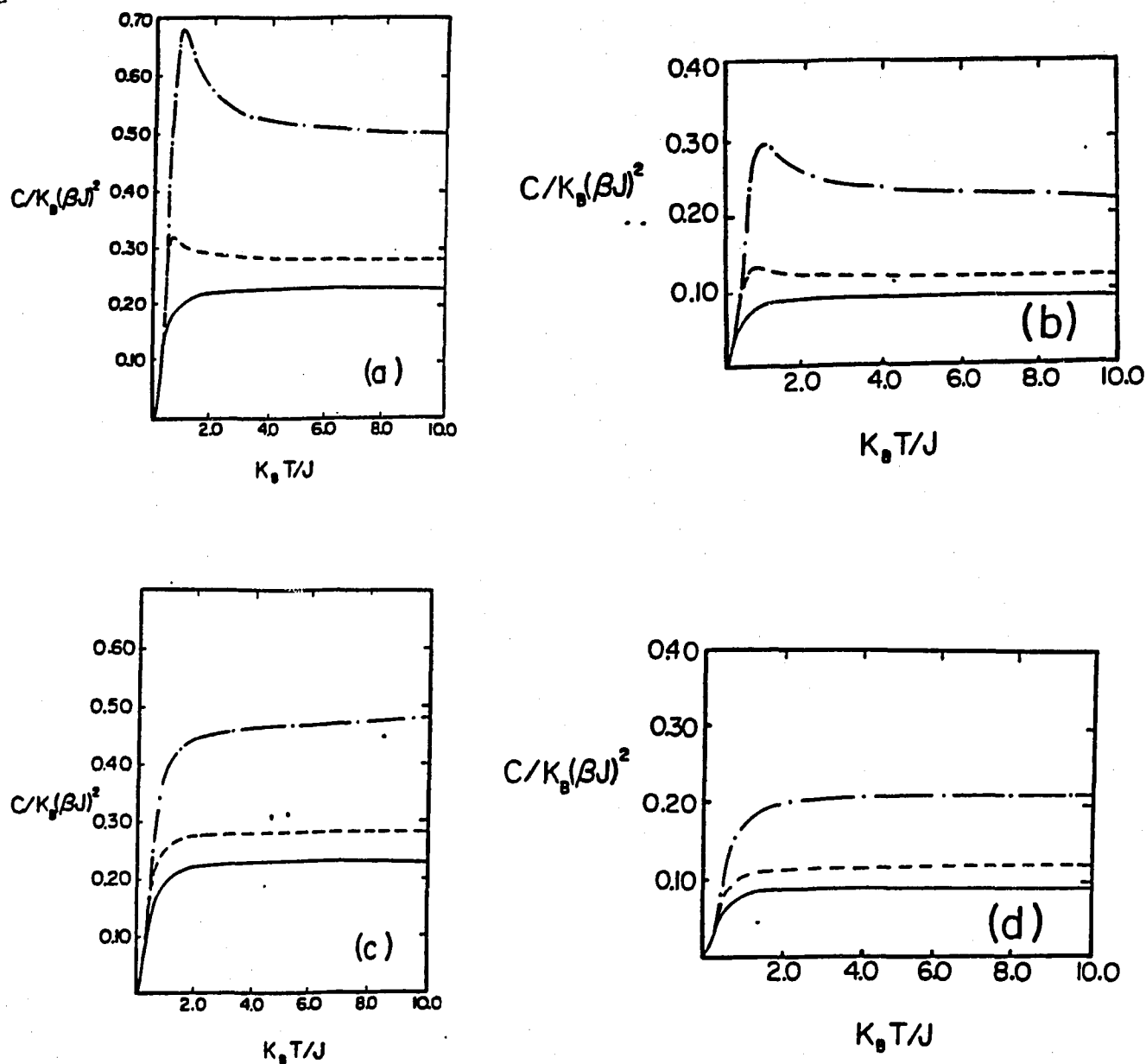


Figure 2. Ferromagnetic specific heat per lattice site versus $k_B T/J$ for $D/J = 2.0$ (dot-dashed), 1.0 (dashed) and 0.5 (solid) for (a) $p = 0.8$, (b) $p = 0.5$. Curves for $D/J = -2.0$ (dot-dashed), -1.0 (dashed) and -0.5 (solid) for (c) $p = 0.8$ and (d) $p = 0.5$

Table 1
Ferromagnetic Energy and Specific Heat

P	D/J	E/J (calculated)	E/J (computer)	C/k(β J) ² (calculated)	C/k(β J) ² (computer)
0.8	0.5	-.1333	-.1562	.2311	.2300
	1.0	-.2667	-.2948	.3844	.2827
	2.0	-.5333	-.5830	.4978	.4978
	-0.5	.1333	.1101	.2311	.2297
	-1.0	.2667	.2380	.2844	.2801
	-2.0	.5333	.4835	.4978	.4769
0.5	0.5	-.0833	-.0928	.0944	.0918
	1.0	-.1667	-.1795	.1278	.1180
	2.0	-.3333	-.3598	.2611	.2250
	-0.5	.0833	.7390	.0944	.0917
	-1.0	.1667	.1539	.1278	.1167
	-2.0	.3333	.3076	.2611	.2146

bigger, while for the negative values the susceptibility tends to approach zero. On the other hand, the curves for x- and y-directions show an opposite character where the susceptibility for positive anisotropy tends to approach zero and the other way around for the negative values. At high temperatures, all the curves seem to approach the correct high temperature limit where $k_{\beta}TX/\mu^2 = p/3$.

For antiferromagnetic coupling, the susceptibility tends to decrease as the temperature is lowered except at the very

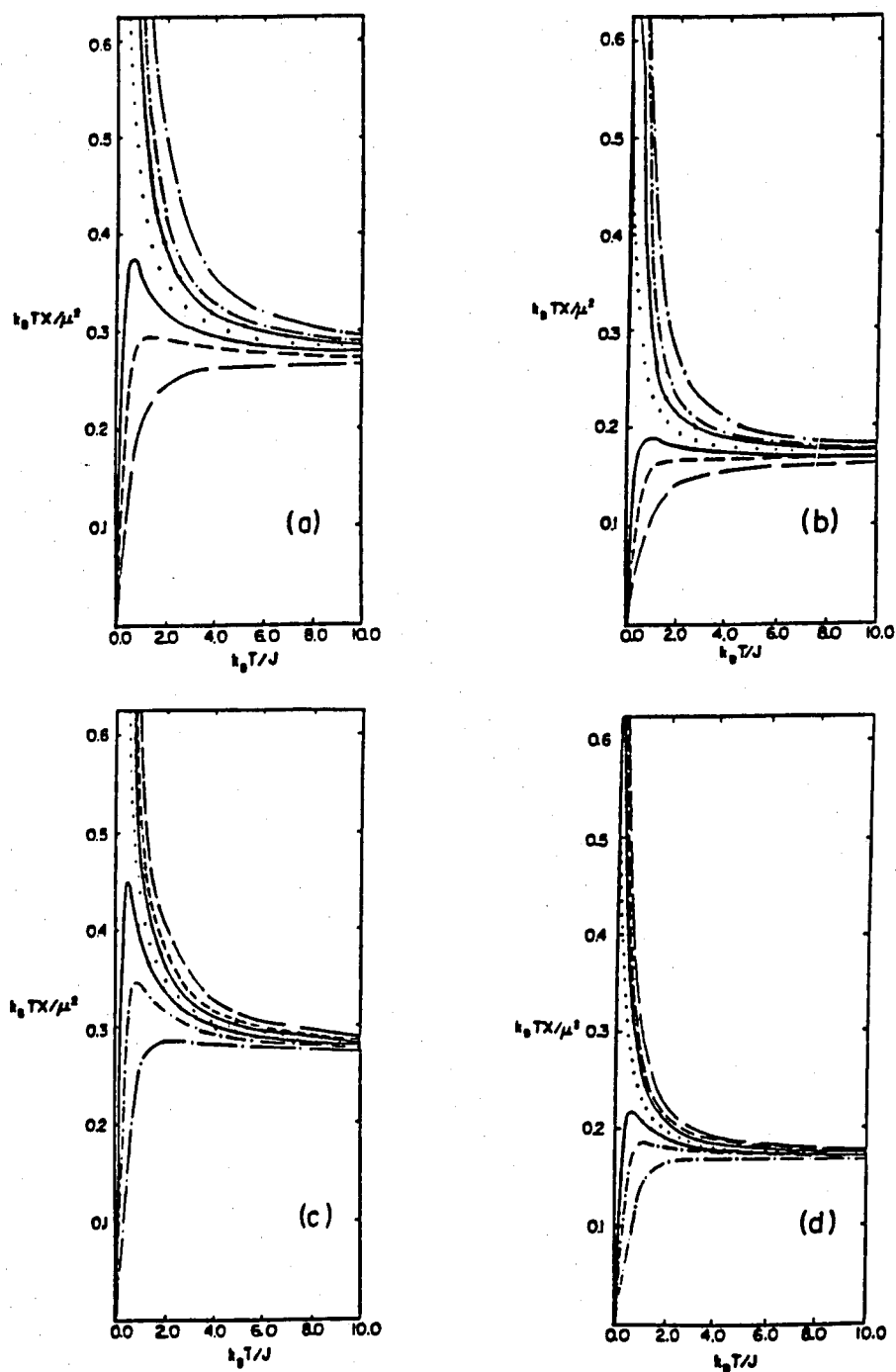


Figure 3. Zero field ferromagnetic susceptibility per lattice site versus $k_B T/J$ for fields along the z-axis in (a) $p = 0.8$, (b) $p = 0.5$ and fields along the x-axis in (c) $p = 0.8$, (d) $p = 0.5$. Curves for $D/J = 2.0$ (long dash-dot), 1.0 (short dash-dot), 0.5 (solid-dot), 0.0 (dotted), -0.5 (solid), -1.0 (short-dashed) and -2.0 (long dashed).

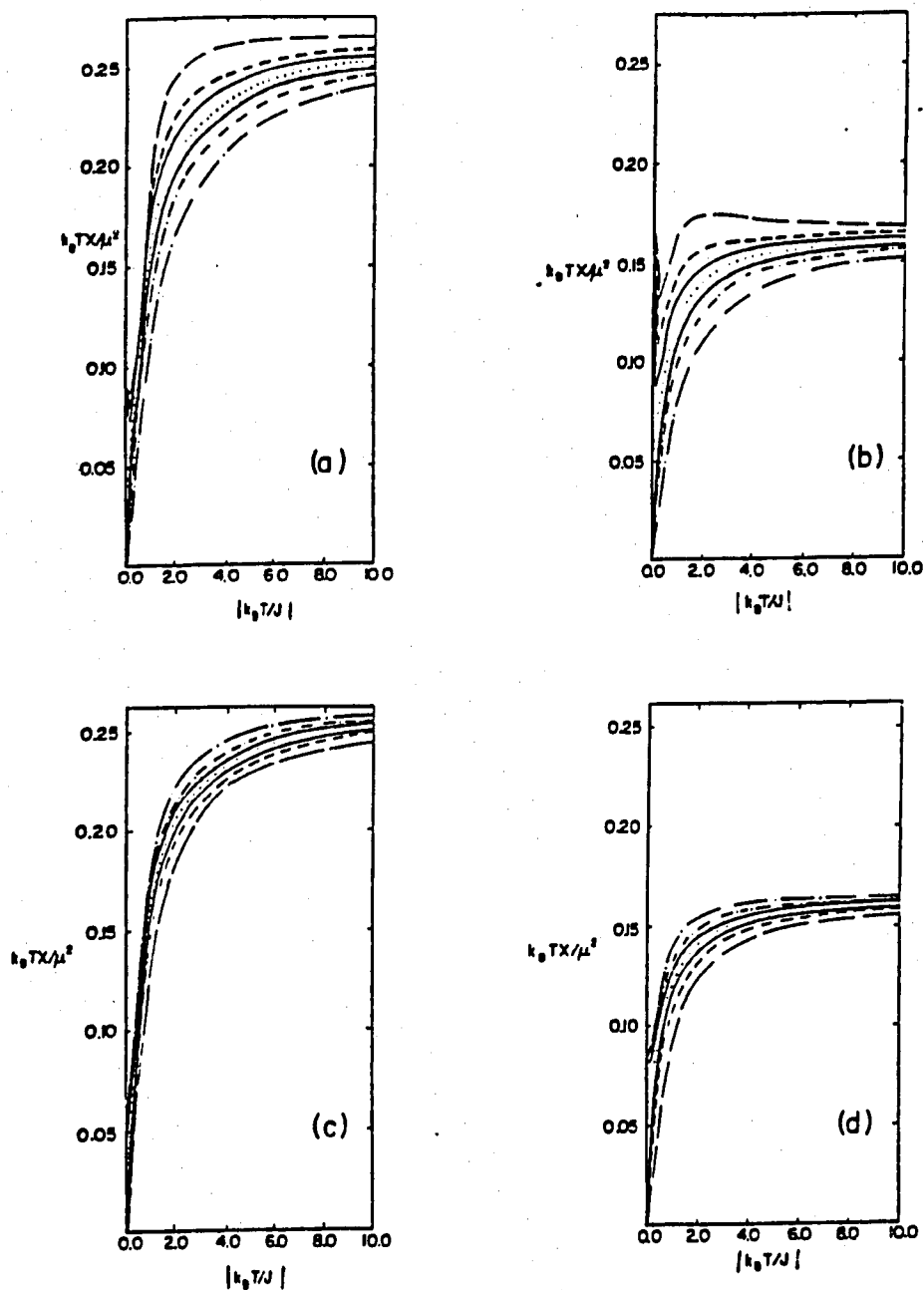


Figure 4. Zero field antiferromagnetic susceptibility per lattice site versus $k_B T/J$ for fields along the z-axis in (a) $p = 0.8$, (b) $p = 0.5$ and fields along the x-axis in (c) $p = 0.8$, (d) $p = 0.5$. Curves for $D/J = -2.0$ (long-dashed), -1.0 (short-dashed), -0.5 (solid), 0.0 (dotted), 0.5 (solid-dotted), 1.0 (short dash-dot), 2.0 (long dash-dot).

Table 2
Ferromagnetic Susceptibility (z-axis)

P	D/J	$k_B T x / \mu^2$ (calculated)	$k_B T x / \mu^2$ (computer)
$\frac{T \rightarrow 0}{0.8}$	2.0	$p(1+p)/(1-p) = 7.20$	6.8316
	1.0		6.6455
	0.5		6.3566
	-2.0	0	0.0203
	-1.0		0.0410
	-0.5		0.0831
0.5	2.0	$p(1+p)/(1-p) = 1.50$	1.4389
	1.0		1.3908
	0.5		1.3053
	-2.0	0	0.0126
	-1.0		0.0254
	-0.5		0.0509
$\frac{T \rightarrow \infty}{0.8}$	2.0	$p/3 = 0.2667$	0.2971
	1.0		0.2889
	0.5		0.2849
	-2.0		0.2665
	-1.0		0.2731
	-0.5		0.2770
0.5	2.0	$p/3 = 0.1667$	0.1820
	1.0		0.1771
	0.5		0.1747
	-2.0		0.1630
	-1.0		0.1676
	-0.5		0.1700

Table 3
Ferromagnetic Susceptibility (x-axis)

P	D/J	$k_B T X / \mu^2$ (calculated)	$k_B T X / \mu^2$ (computer)
$\frac{T \rightarrow 0}{0.8}$	2.0	0	0.0204
	1.0		0.0415
	0.5		0.0856
	-2.0	$p(1+p)/2(1-p) = 3.600$	2.6975
	-1.0		2.6559
	-0.5		2.5933
0.5	2.0	0	0.0128
	1.0		0.0262
	0.5		0.0553
	-2.0	$p(1+p)/2(1-p) = 0.7500$	0.6858
	-1.0		0.6743
	-0.85		0.6551
$\frac{T \rightarrow \infty}{0.8}$	2.0	$p/3 = 0.2667$	0.2729
	1.0		0.2769
	0.5		0.2789
	-2.0		0.2887
	-1.0		0.2848
	-0.5		0.2829
0.5	2.0	$p/3 = 0.1667$	0.1675
	1.0		0.1699
	0.5		0.1711
	-2.0		0.1770
	-1.0		0.1747
	-0.5		0.1735

Table 4

Antiferromagnetic Susceptibility (z-axis)

P	D/J	$k_p TX/\mu^2$ (calculated)	$k_p TX/\mu^2$ (computer)
$\frac{T \rightarrow 0}{0.8}$	2.0	0	0.0116
	1.0		0.0168
	0.5		0.0227
	-2.0	$p(1-p)/(1+p) = 0.0889$	0.0918
	-1.0		0.0879
	-0.5		0.0808
0.5	2.0	0	0.0089
	1.0		0.0148
	0.5		0.0236
	-2.0	$p(1-p)/(1+p) = 0.1667$	0.1584
	-1.0		0.1499
	-0.5		0.1318
$\frac{T \rightarrow \infty}{0.8}$	2.0	$p/3 = 0.2667$	0.2410
	1.0		0.2462
	0.5		0.2493
	-2.0		0.2655
	-1.0		0.2590
	-0.5		0.2557
0.5	2.0	$p/3 = 0.1667$	0.1530
	1.0		0.1571
	0.5		0.1591
	-2.0		0.1697
	-1.0		0.1654
	-0.5		0.1633

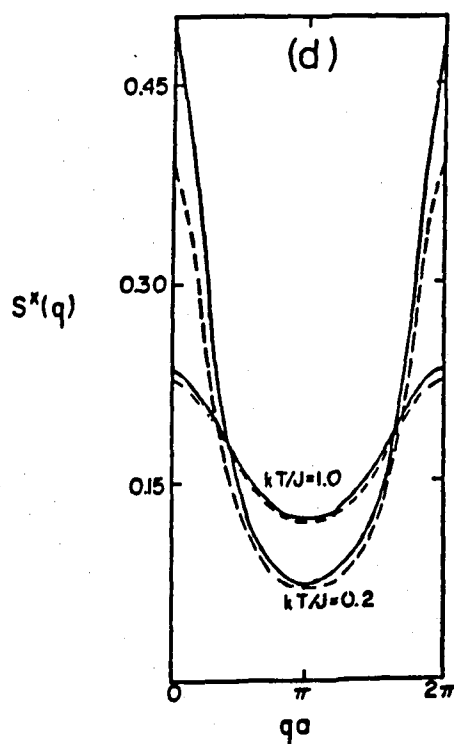
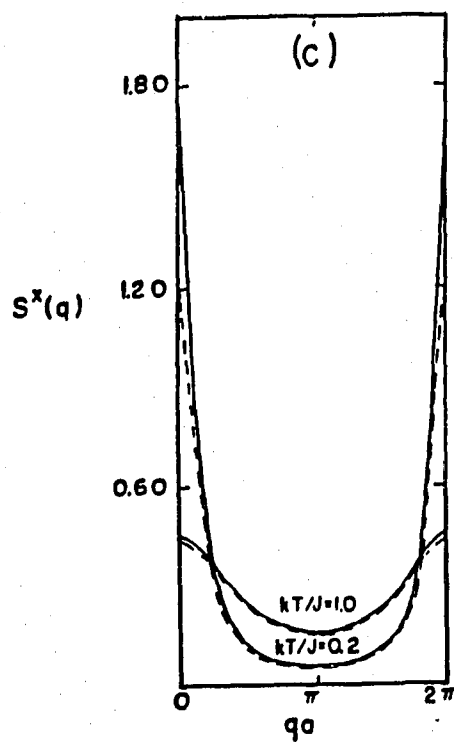
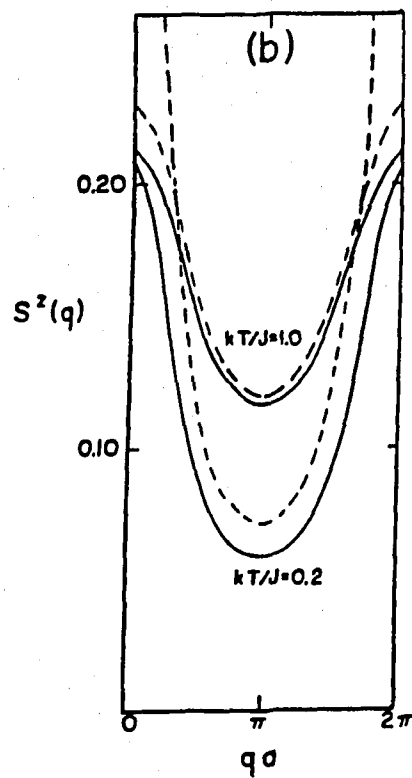
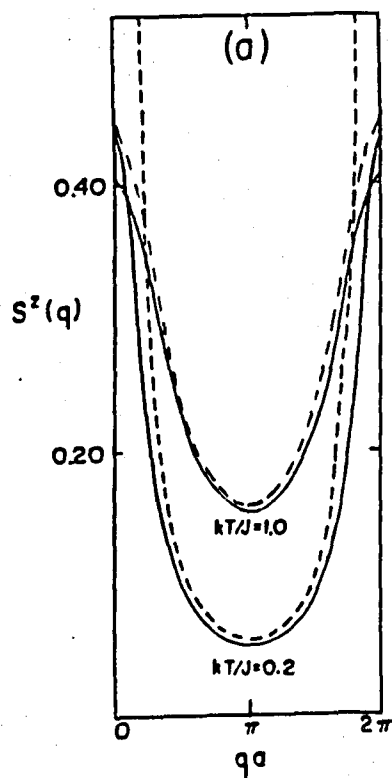
Table 5
Antiferromagnetic Susceptibility (x-axis)

P	D/J	$k_B T X / \mu^2$ (calculated)	$k_B T X / \mu^2$ (computer)
$\frac{T \rightarrow 0}{0.8}$	2.0	$p(1-p)/2(1+p) = 0.0444$	0.0550
	1.0		0.0541
	0.5		0.0527
	-2.0	0	0.0116
	-1.0		0.0171
	-0.5		0.0236
0.5	2.0	$p(1-p)/2(1+p) = 0.0834$	0.0871
	1.0		0.0852
	0.5		0.0817
	-2.0	0	0.0263
	-1.0		0.0153
	-0.5		0.0095
$\frac{T \rightarrow \infty}{0.8}$	2.0	$p/3 = 0.2667$	0.2588
	1.0		0.2557
	0.5		0.2541
	-2.0		0.2460
	-1.0		0.2493
	-0.5		0.2509
0.5	2.0	$p/3 = 0.1667$	0.1653
	1.0		0.1633
	0.5		0.1622
	-2.0		0.1570
	-1.0		0.1591
	-0.5		0.1602

low temperature, where it increases for negative anisotropy for the z-direction and positive for the x- and y-directions.

Finally the graph of neutron scattering versus wave vector are plotted in Figures 5a through 5d for the ferromagnetic case with $kT/J = 1.0$ and 0.2 for both isotropic and anisotropic systems. The parameter D/J used for the anisotropic system is $-4.5/23.6$ which is appropriate to the systems formed from CsNiF_3 at low temperature. It can be seen that for the z-direction, the values for the isotropic system are bigger than for the anisotropic system, while for the x- and y-directions the opposite case happens.

Figure 5. Plot of $S^l(q)$ versus qa for $l = x$ and z and $kT/J = 0.2$ and 1.0 . Curves for $S^z(q)$ with in (a) $p = 0.8$ and (b) $p = 0.5$ where $D/J = -0.1907$ (solid) and $D/J = 0.0$ (dashed). Curves for $S^x(q)$ with in (c) $p = 0.8$ and (d) $p = 0.5$ where $D/J = -0.1907$ (solid) and $D/J = 0.0$ (dashed).



CHAPTER IV

CONCLUSIONS

In this study, the thermodynamics and magnetic properties of the disordered materials in the absence of an external field are calculated and comparisons are made between the results obtained with the low and high temperature limits. In all the cases except for the neutron scattering, calculations are made for both systems, ferromagnetic and antiferromagnetic. In addition, for the magnetic susceptibility and neutron scattering, both isotropic and anisotropic systems are considered. The plots which represent the results for magnetic concentration $p = 0.8$ and 0.5 are presented.

This study is interesting because the phenomena happens in the real system for compounds formed from CsNiF_3 and TMMC. It was shown also, that the thermodynamics of the diluted classical spin Heisenberg chain with single ion anisotropy can be solved exactly in one dimension based on the classical models.

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