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Full Length Research Paper

The magnetic behaviour of an isolated paramagnetic spin-1 and spin-1/2 degree of freedom

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The effect of external magnetic field and temperature on paramagnetic spin-1/2 and spin-1 degree of freedom was investigated. Magnetization *m(h,T)* and magnetic susceptibility are found to have a direct and inverse behaviour with external magnetic field and temperature respectively. Various limiting cases of *m(h,T)* were considered for different temperatures and external magnetic field. The agreement with Curie's law was observed. The saturated points of m(h,T) for spin-1 and spin-1/2 are discussed. Comparison between magnetic susceptibility of spin-1/2 and spin-1 as a function of temperature was also examined.

Key words: Paramagnetism, spin degrees of freedom, magnetization and magnetic susceptibility.

INTRODUCTION

The Heisenberg Hamiltonian is a quantum mechanical analogue of the Ising model (for an introduction sees (Manousakis, 1991; Affleck, 1988), an early discussion can be found in (Van Vleck, 1932)).This model is a variant of the Hubbard model (Hubbard, 1963) at half filling and large onsite Coulomb repulsion U, which enforces the constraint of singly occupied site. The model, describing the pairwise interactions between localized spins, is one of the most fundamental models of correlated quantum matter. In spite of its simple mathematical form, it has an unimaginable richness, arising from dimensionality and geometrical constraints, competing exchange interaction, the type of spin degrees of freedom and additional interactions with external magnetic fields or other degrees of freedom such as phonons.

Neutron scattering experiments (Shirane et al., 1989; Aeppli et al., 1989) show that the magnetic behaviour of materials is well described by the quantum Heisenberg models. Following the PhD Thesis of Pierre Curie (Paris: Gautheir-Villars; 1895) (Curie, 1895), there have been oodles of theoretical and experimental research on the dependence of paramagnetic materials and its variants on magnetic field and temperature. Temperature dependence of the so-called two-magnon excitation in the paramagnetic phase was studied by using the "Equation-of-Motion Method" (Horsch and von der, 1988). Here, the temperature variations of frequency shift, absorption coefficient and integrated intensity were found to coincide with experimental data. The investigation of the ground state and the lowest excited state of the spin 1/2-heisenberg model using ED and VMC was carried out by Horsch and von der (1988). Their calculation on the dispersion of spin-wave excitation revealed an excited triplet which becomes degenerate with the ground state in the thermodynamic limit. A study of spontaneous magnetization as a function of temperature by Xuang-Zhang *and* Zhan Zhang 1990, (Masahiko et al., 2002) found the existence of multiple magnetism in the super-lattices. A Universal electron paramagnetic resonance (EPR) simulation program developed by Hanqing Wu 1996; (Larico, 2004) was used for the simulation of EPR spectra of spin-1 and spin-1/2. The EPR simulation results show the absence of EPR signal in the EPR simulation when *D* > frequency and the presence of an EPR signal, when *D* ≈ frequency. From synthesized powder sample of $NaTiSi_2O_6$, Masahiko et al. (2002) observed a typical behaviour of magnetic susceptibility in a spin-1/2 1D magnet, followed by a spin-Peierls-like transition at 210 K. Furthermore, a study of electronic properties and structural properties of isolated nickel impurities in diamond was in agreement \with EPR model and optical experiments on synthetically grown diamond Larico Braz R (2004). More recently, paramagnetic results on one-dimensional spin-1 single-ion studied by the random phase approximation for the exchange interaction term and the Anderson–Callen approximation for the anisotro-

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py term were found to be in agreement with the other theoretical results (Hai-Jun et al., 2009).

A fundamental starting point in the study of the magnetic property of undoped materials is the study of magnetic property of a single isolated spin. This system, though deceitfully simple is the key for probing into more complex systems. This paper, therefore, focuses on the detailed study of isolated spin-1 and spin-1/2 degree of freedom of a paramagnet and their response to external magnetic field and temperature.

The layout of this paper is as follows. In the next section, we present the Heisenberg Hamiltonian and reformulate it in terms of creation and annihilation operators. In subsequent section, a detailed study of spin-1/2 degree of freedom is presented. The effect of temperature and an external magnetic field is elucidated.

Also, detailed examination of spin-1 degree of freedom and its dependence on temperature and an external magnetic field is presented. Graphically comparison on the paramagnetic susceptibility of spin-1/2 and spin-1 degree of freedom is presented in subsequent section. From this, a conclusion in drawn.

THE HEISENBERG HAMILTONIAN

For the case where the pairwise interactions between the spins are isotropic, the basic Heisenberg Hamiltonian is commonly represented as

$$H = \sum_{i,j} J_{ij} S_i . S_j - h \sum_i S_i \quad (1)$$

Where; J_{ij} the exchange integrals between spins are on sites *i* and *j* which decays rapidly with distance between these sites. The ground state of the model depends on the sign of the exchange integral. If J_{ij} >0 (antiferromagnetic alignment), the ground is the checker board-like Neel state, with all the spins up at the even sites and down at the odd site or the other way round. If J_{ij} <0 (ferromagnetic alignment), the spins tend to align themselves with their neighbour and the ground state is the configuration with either all the spins up or all down. More often, only nearest-neighbour interactions are considered and longer-range interactions are neglected. The spin operators S_i represent quantum spin degrees of freedom, that is with S= ½ or 1. h represents an applied external magnetic field. Additional richness enters the Hamiltonian when anisotropies are considered. For example, a frequently studied variant of the isotropic Heisenberg model is the XYZ model. With $S_i . S_j \rightarrow \lambda S_i^z S_j^z + S_i^x S_j^x + S_i^y S_j^y$, where the anisotropy parameter λ interpolates between the XY limit ($\lambda = 0$), the Heisenberg limit ($\lambda = 1$) and the Ising limit ($\lambda = \infty$). The spin operators $S_i . S_j$ for the Heisenberg limit can be written as;

$$S_i . S_j = S_i^z S_j^z + S_i^x S_j^x + S_i^y S_j^y \quad (2)$$

Where;

$$S_i^x S_j^x + S_i^y S_j^y = \tfrac{1}{2}(S_i^+ . S_j^- + S_i^- . S_j^+) \quad (3)$$

In terms of creation and annihilation operators, the spin operators are defined as;

$$\left.\begin{aligned} S_i^+ &= C_{i\uparrow}^+ C_{i\downarrow} \\ S_i^- &= C_{i\downarrow}^+ C_{i\uparrow} \\ S_i^z &= \tfrac{1}{2}(n_{i\uparrow} - n_{i\downarrow}) \end{aligned}\right\} \quad (4)$$

Where;

$$n_{i\sigma} = C_{i\sigma}^+ C_{i\sigma} \quad (5)$$

Using equation (2 - 5), the Hamiltonian (1) for the Isotropic Heisenberg antiferromagnetic is given by

$$H = H_Z + H_{XY} + H_h \quad (6)$$

These quantities are defined by;

$$H_h = \frac{h}{2} \sum_i \left[C_{i\uparrow}^+ C_{i\uparrow} - C_{i\downarrow}^+ C_{i\downarrow} \right] \quad (7)$$

$$H_{XY} = \frac{J}{2} \sum_{\langle i,j \rangle} \left[C_{i\uparrow}^+ C_{i\downarrow} C_{j\downarrow}^+ C_{j\uparrow} + C_{i\downarrow}^+ C_{i\uparrow} C_{j\uparrow}^+ C_{j\downarrow} \right] \quad (8)$$

$$H_Z = \frac{J}{4} \sum_{\langle i,j \rangle} \begin{bmatrix} C_{i\uparrow}^+ C_{i\uparrow} C_{j\uparrow}^+ C_{j\uparrow} - C_{i\uparrow}^+ C_{i\uparrow} C_{j\downarrow}^+ C_{j\downarrow} - C_{i\downarrow}^+ C_{i\downarrow} C_{j\uparrow}^+ C_{j\uparrow} \\ + C_{i\downarrow}^+ C_{i\downarrow} C_{j\downarrow}^+ C_{j\downarrow} \end{bmatrix} \quad (9)$$

ISOLATED SPIN ½ DEGREE OF FREEDOM

In this session, we consider the response of a single quantum spin-1/2 to an applied magnetic field.Spin-1/2 degree of freedom has projection of ± 2 along the z-axis. The Hilbert space of this system has two states $|\uparrow\rangle$ and $|\downarrow\rangle$. Since there is no interaction, the only relevant part of H in equation 6 is H_h. Hence, the Hamiltonian of this system is given by:

$$H_h = -\frac{h}{2} \sum_i \left[C^+_{\uparrow} C_{\uparrow} - C^+_{\downarrow} C_{\downarrow} \right] \quad (10)$$

Table 1. Variation of m(h,T) with h for fixed values of T

H	T=0.2 m_1 (h,T)	T=0.6 m_1 (h,T)	T=1 M_3 (h,T)	T=1.2 m_4 (h,T)
0.00	0.000000000	0.000000000	0.000000000	0.000000000
0.5	0.42414182	0.19705928	0.12245933	0.10268534
1	0.49330715	0.3411309	0.23105858	0.19705928
1.5	0.49944722	0.42414182	0.31757448	0.27729986
2	0.4999546	0.4655548	0.38079708	0.3411309
2.5	0.49999627	0.48473285	0.42414182	0.38927268
3	0.49999969	0.49330715	0.45257413	0.42414182
3.5	0.49999997	0.49708025	0.47068777	0.44866421
4	0.50000000	0.49872898	0.48201379	0.4655548
5	0.50000000	0.49975969	0.49330715	0.48473285

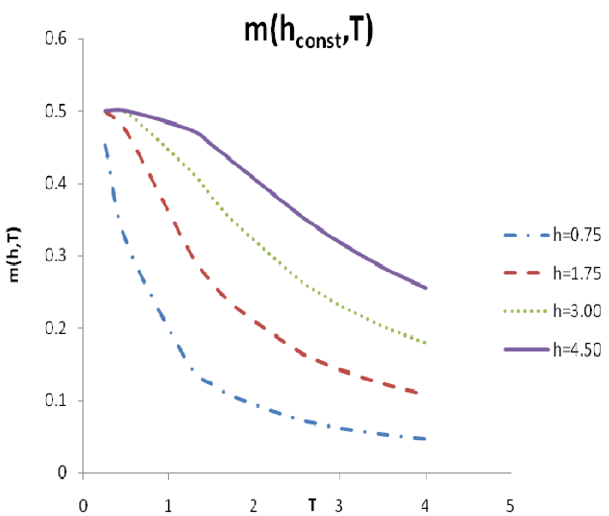

Figure 1. A plot of m(h,T) versus h for fixed values of T.

The action of H on these two states will generate a diagonalized 2x2 matrix as shown below

$$H_{ij} = \begin{bmatrix} -\frac{h}{2} & 0 \\ 0 & \frac{h}{2} \end{bmatrix} \quad (11)$$

The matrix is already diagonal with ground state energy given by $E_g = -\frac{h}{2}$ and excited state given by $E_{ex} = \frac{h}{2}$.

The magnetization of this system is given by;

$$m(h,T) = \frac{\sum_i S_i \exp(-\beta E_i)}{\sum_i \exp(-\beta E_i)} = \frac{1}{2}\frac{Sinh\left(\frac{\beta}{2h}\right)}{Cosh\left(\frac{\beta}{2h}\right)} = \frac{1}{2} Tanh\left(\frac{\beta}{2h}\right)$$

12)

The magnetic susceptibility $\chi(T)$ of this system is obtained by taking the partial derivative of m (h, T*)* with respective to *h* at the limit $h \to 0$ .Hence, we have that

$$\chi(T) = \left.\frac{\partial m(h,T)}{\partial h}\right|_{h=0} = \frac{\beta}{4} Sech^2\left(\frac{\beta h}{2}\right)\Big|_{h=0} = \frac{\beta}{4} \quad (13)$$

This result shows the inverse dependence of magnetic susceptibility and magnetization on temperature (Curie's law).

GRAPHICAL AND PHYSICAL INTERPRETATION OF $m(h,T)$

Since the magnetization of this system is a function of both temperature and magnetic field, to visualize its physical content, it is necessary that to plot it against h and T for given values of T and h, respectively (Table 1 and 2).

In Figure 1, as $h \to 0$, $m(h,T) \to 0$, for any value of T. In this limit, $\beta h/2 \to 0$ and $Tanh\left(\frac{\beta h}{2}\right) \to \beta h/2$. In Figure 2, as $T \to 0$ or $\beta h/2 >> 1$, $m(h,T) \to 1/2$. In this limit, $Tanh\left(\frac{\beta h}{2}\right) \to 1$. Also, in Figure 2, for given value of T, the function m (h, T) is observed to be nearly parallel to h axis (indicating zero gradient) as the value of h is increased. This behaviour indicates that m (h, T) has attained its saturated value of 0.5

ISOLATED DEGREES SPIN-1 OF FREEDOM

Spin-1 degrees of freedom has projections 1, 0, -1, along

Table 2. Variation of m (h, T) with T for fixed values of h.

T	h=0.75 m_1(h,T)	h=1.75 m_2(h,T)	h=3 m_3(h,T)	h=4.5 m_4(h,T)
0.25	0.45257413	0.49908895	0.49999386	0.49999998
0.50	0.31757448	0.47068777	0.49752738	0.49987661
1.25	0.14565631	0.30218389	0.4168273	0.47340301
1.50	0.12245933	0.26254197	0.38079708	0.45257413
1.75	0.10553249	0.23105858	0.34739134	0.42899998
2.50	0.07444252	0.16818777	0.26852478	0.35814894
2.75	0.06776232	0.15393099	0.24855287	0.33703953
3.00	0.0621765	0.14183405	0.23105858	0.31757448
3.50	0.05336737	0.12245933	0.20206337	0.28342090
4.00	0.04673815	0.10766317	0.1791787	0.25491499

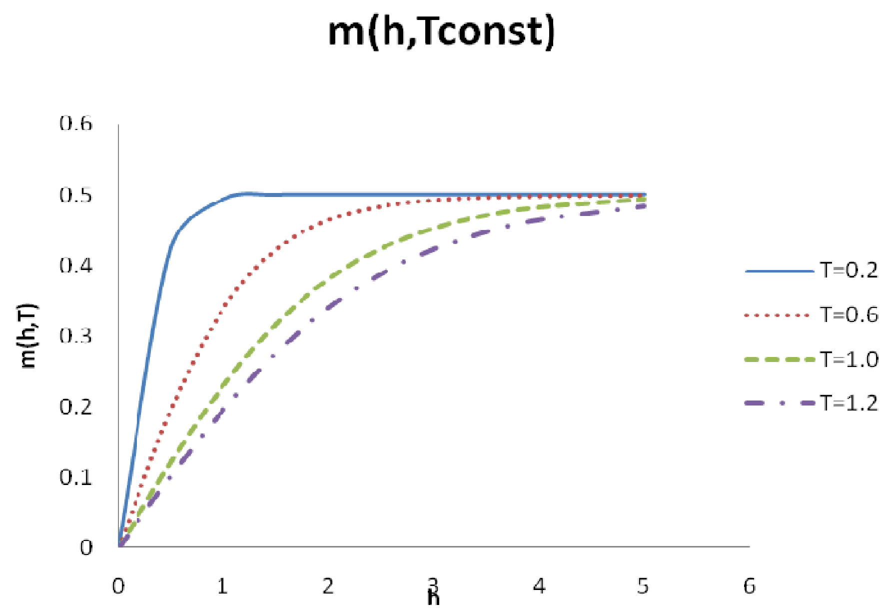

Figure 2. A plot of m (h,T) versus T for fixed values of h.

the direction of z-axis. The size of the Hilbert space of this system is 3 that is, $\uparrow$, $\downarrow$ and 0.These three projections will give rise to the eigenvalues 0,-h and h. The magnetization of this system is giving by:

$$m(h,T)=\frac{\exp(\beta h)-\exp(-\beta h)}{\exp(\beta h)-\exp(-\beta h)+1}=\frac{2Sinh(\beta h)}{1+2Cosh(\beta h)} \quad (14)$$

The derivative of magnetization with respect to the applied field gives

$$\frac{\partial(m(h,T))}{\partial h}=\frac{2\beta Cosh(\beta h)}{1+2Cosh(\beta h)}-\frac{4\beta Sinh(\beta h)^2}{[1+2Cosh(\beta h)]^2} \quad (15)$$

The susceptibility of the system is given by;

$$\chi(T)=\left.\frac{\partial(m(h,T))}{\partial h}\right|_{h=0}=\frac{2\beta}{3} \quad (16)$$

This result for spin-1 degree of freedom still obeys the Curie's law for isolated spin.

GRAPHICAL INTERPRETATION OF SPIN-1 DEGREE OF FREEDOM

It is useful to visualize the physical content of m (h, T) by plotting it against temperature and magnetic field for given values of magnetic field and temperatures respectively (Tables 3 and 4). In Table 3, there exist a linear relationship between m (h, T) and h for given values of T and for Table 4, an inverse relationship exists between m (h, T) and T for given values of h.

Table 3. The different values of m (h, T) obtained by slightly varying h for given values of T. In this table, there exist a linear relationship between m (h, T) and h for given values of T.

H	T = 0.2 $m_1(h,T)$	T = 0.6 $m_2(h,T)$	T = 1 $m_3(h,T)$	T = 1.2 $m_4(h,T)$
0.00	0.00000000	0.00000000	0.000000000	0.00000000
0.5	0.91223468	0.49962272	0.32015667	0.27003119
1.0	0.99321726	0.78749445	0.57521038	0.49962272
1.5	0.99944661	0.91223468	0.74648446	0.67070133
2.0	0.9999546	0.9631425	0.85093709	0.78749445
2.5	0.99999627	0.98426317	0.91223468	0.86357923
3.0	0.99999969	0.99321726	0.94797458	0.91223468
3.5	0.99999997	0.99706318	0.96894495	0.94326587
4.0	1.00000000	0.99872575	0.98136107	0.9631425

Table 4. Values of m (h, T) are obtained by varying T for given values of h. An inverse relationship exists between m (h, T) and T for given values of h.

T	h = 0.75 $m_1(h,T)$	h = 2 $m_2(h,T)$	h = 3.5 $m_3(h,T)$	h = 5 $m_4(h,T\}$
0.25	0.94797458	0.99966442	0.99999917	1.00000000
0.50	0.74648446	0.98136107	0.99908729	0.9999546
1.25	0.37773166	0.77192376	0.9359274	0.98136107
1.50	0.32015667	0.69801973	0.89535281	0.9631425
1.75	0.27730217	0.63233393	0.85093709	0.93963632
2.50	0.19705734	0.4833401	0.71836078	0.85093709
2.75	0.17959996	0.4464842	0.67836569	0.81911142
3.00	0.16495374	0.41440459	0.64118428	0.78749445
3.50	0.14177461	0.3615866	0.57521038	0.72668203
4.00	0.12427311	0.32015667	0.51943127	0.67070133

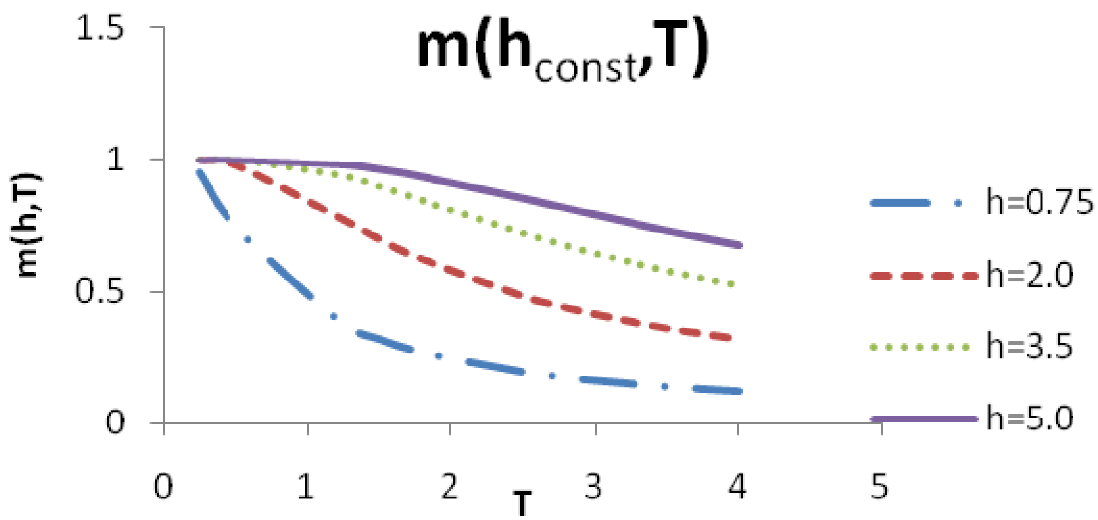

Figure 3. A plot of m (h,T) versus T for varying values of h.

Figure 3 shows that for a given temperature, the magnetization increases with increasing magnetic field, saturating at its maximum value of 1. In Figure 4, the relationship between m (h, T) and T for given values of h is inverse. For both graphs, when the argument (βh) is extremely large or small, the magnetization for spin-1

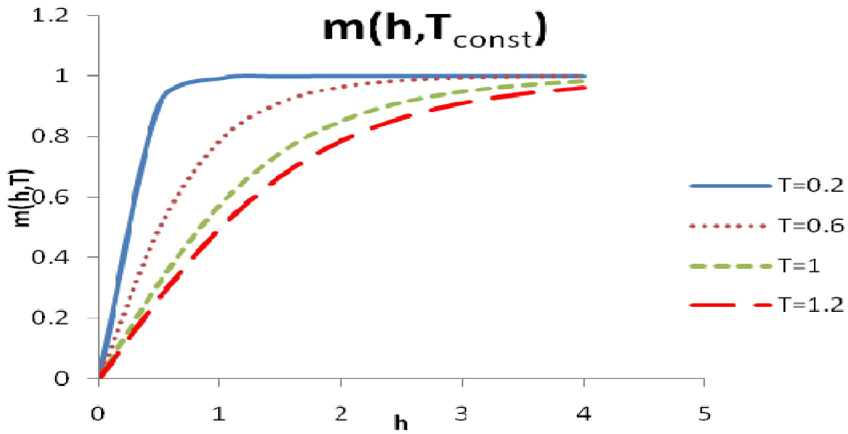

Figure 4. The inverse relationship between m (h,T) and T for given values of h.

Table 5. The inverse behaviour of (T) for both spin-1 and spin-1/2 systems as a function of temperature.

T	Spin-1/2 (χ)	Spin-1 (χ)
0.25	1.0000	2.66666667
0.50	0.5.000	1.33333333
1.25	0.2000	0.53333333
1.50	0.1667	0.44444444
1.75	0.1429	0.38095238
2.50	0.1000	0.26666667
2.75	0.0909	0.24242424
3.00	0.0833	0.22222222
3.50	0.0714	0.19047619
4.00	0.0625	0.16666667

degree of freedom takes the form

$$m(h,T) = Tanh\ (\beta h) \quad (17)$$

This implies that the zero temperature and magnetic field magnetization are 1 and 0 respectively.

MAGNETIC SUSCEPTIBILITY OF SPIN-1/2 AND SPIN-1

Magnetic susceptibility χ for both spin-1 and spin-1/2 degree of obeys the inverse law. This inverse relationship between χ and T, clearly suggests that an increase in thermal energy of the system will lead to a decrease in χ (Table 5).

From both graph (Figure 5), the magnetic susceptibility increases with decrease in temperature. Another important observation from the graph is that the magnetic susceptibility for spin-1 degree of freedom is greater than spin-1/2 degree of freedom for the same range of temperatures. This implies that the thermal agitation in response to temperature is more in spin-1/2 compared to spin-1

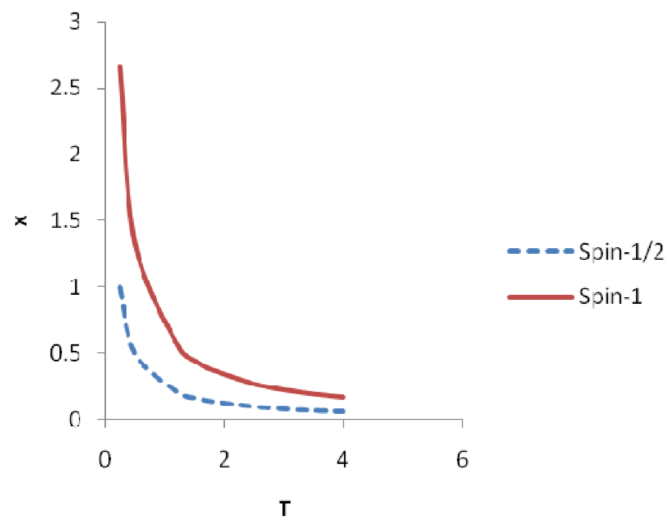

Figure 5. Plot of χ (T) versus T for both spin-1/2 and spin-1.

Conclusion

In this paper, we have examined two cases of paramagnetism, that of spin-1/2 and spin-1 degree of freedom. For both systems, magnetization and susceptibility are affected by temperature and magnetic field in accordance with Curie's law. The plot of m (h, T) against h, for given values of temperature and vice versa, shows that the saturated values of m (h, T) for spin-1/2 and spin-1 are respectively ½ and 1. An important observation in this work is that besides temperature and magnetic field, the magnetization and susceptibility also depend on the spin degree of freedom. The comparison between magnetic susceptible of spin-1/2 and spin-1 shows that spin-1 systems have the tendency to sustain magnetism more than spin-1/2 systems for the same range of temperatures. In general, the tendency of atomic magnetic moments to align themselves parallel to magnetic field (were the potential is minimum) is opposed by random thermal motion which tends to randomize their orientations. For this reasons, paramagnetic susceptibility and magnetization always decreases with increasing temperature.

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