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The Study of Magnetic Properties of $A_{1-x}Mn_xA'(A = Zn, Cd$ and $A' = S, Te, Se)$ at Critical Region Using High Temperature Series Expansion Extrapolated with PAD$\acute{E}$ Approximants

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Authors' contributions

The corresponding author HDB designed the study, manuscript preparation and all mathematical and numerical calculations. Author PS read and approved the manuscript.

Research Article

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ABSTRACT

Aims: In the present work we explore magnetic properties especially spin glass, antiferromagnetic and paramagnetic states of diluted magnetic semiconductors $\left(A_{1-x}Mn_xA'(A = Zn, Cd \text{ and } A' = \text{S, Te, Se})\right)$.
Place: Department of physics, College of natural sciences, Addis Ababa University, between Sept. 2012, and May 2013.
Methodology: Using classical Heisenberg model with high temperature series expansion extrapolated with pad*é* approximants.
Results: Different magnetic phases using different concentration regions
Conclusion: We used high temperature series expansion extrapolated with pad*é* approximants to determine the critical temperature (T_c), exchange interaction couplings, critical exponents of magnetic susceptibility and correlation function.

Keywords: Diluted magnetic semiconductors (DMSs); Heisenberg model; High temperature series expansion (HTSE); PADé approximants.

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1. INTRODUCTION

There are several classes of semiconducting materials that are characterized by the random replacement of a fraction of the original atoms by magnetic atoms. The materials are usually known as diluted magnetic semiconductors (DMSs) or semi-magnetic semiconductors (SMSCs).The first so-called diluted magnetic semiconductors were IIB-VI semiconductor alloys like $Zn_{1-x}Mn_xTe$ and $Cd_{1-x}Mn_xTe$ [1] originally studied in the 1980s. These materials are either spin glasses or have very low ferromagnetic (FM) critical temperatures T_c (~ few K) [2] and are, therefore, inadequate for technological applications which would require FM order at room temperature. It's obvious that, the possibility of using the spin and the charge of the electrons for information processing will have numerous applications in recent technology. The DMS materials can be considered as consisting of two interacting subsystems. The first one of these subsystems is the system of delocalized conduction or valence band electrons/holes. The second one is the random and diluted system of localized magnetic moments associated with the magnetic atoms. These two subsystems interact with each other by the spin exchange interaction. The coupling between the localized moments result in the occurrence of different magnetic phases such as paramagnets, spin glasses and antiferromagnets.

In this paper, we study spin glass and antiferromagnetic states that exist in IIB-VI semiconductors which consist of S, Te, Se, and of Zn, Cd. The fraction of cation site is replaced with Mn (or Fe) as the magnetic impurity. A prototype of this is $Cd_{1-x}Mn_xTe$. Theoretical studies have shown that super exchange is the basic source of magnetic coupling, i.e., the filled valence band of the semiconductor exchange electrons with the half filled 3d band of the Mn. With this 2 electron process the interaction between the Mn will always lead to an antiferromagnetic interaction and seems to be true for both first and second nearest neighbors [3,4,5]. One of the advantages of IIB-VI materials is that they can host magnetic ions (e.g. Mn^{2+}) which open the way for studying various spin-dependent phenomena.

2. MODELS AND INTERACTION COUPLING CALCULATIONS

We consider Heisenberg spin (vector spin) model. The Hamiltonian [6] will be:-

$$H = -2\sum_{ij} J_1 \boldsymbol{s_i}.\boldsymbol{s_j} - \mathbf{2}\sum_{ik} J_2 \boldsymbol{s_i}.\boldsymbol{s_k}. \qquad \textbf{(}2.1\textbf{)}$$

Where (ij) and (ik) indicate nearest neighbor and next nearest neighbor summations respectively. The vector spin [7,8] can be described as:-

$$\boldsymbol{s_i}.\boldsymbol{s_j} = \mathrm{s_i^x s_j^x} + \mathrm{s_i^y s_j^y} + \mathrm{s_i^z s_j^z}\ \mathbf{,} \qquad (2.2)$$

$$\boldsymbol{s_i}.\boldsymbol{s_k} = \mathrm{s_i^x s_k^x} + \mathrm{s_i^y s_k^y} + \mathrm{s_i^z s_k^z}\ \mathbf{.} \qquad (2.3)$$

For diluted magnetic semiconductors containing the magnetic impurities [9] only in the octahedral sub lattices, by using molecular-field approximation we can obtain the relationship between paramagnetic Curie-temperature (θ_p) and the Neel temperature (T_N), and considered exchange interaction couplings J_1 and J_2. According to Holland and Brown [10]:-

$$T_N = \frac{2s(s+1)}{3k_B}[-4J_1 + 2J_2], \qquad (2.4)$$

$$\theta_p = \frac{2s(s+1)}{3k_B}[12J_1 + 6J_2]. \quad (2.5)$$

Where k_B is the Boltzmann constant and $s = {}^5/_2$ is the spin of magnetic impurity (Mn^{2+}). By using the experimental values of θ_p and T_N [11] we can determine the interaction couplings J_1 and J_2 for the concentrations ($0.6 \leq x \leq 1$). However, due to the nature of dilution problem in the system, we have to use the probability distribution to determine the interaction couplings for each concentration $x(0 \leq x \leq 1)$. The probability of the occupation of the ion (i) can be defined as:-

$$P(i) = K_n^i x^{n-i}(1-x)^i. \quad (2.6)$$

Where n is the total number of lattice sites inside a sphere of radius (r_i) and its volume ($\frac{4}{3}\pi r_i^3$) (r_i is the distance between ions i and j), $K_n^i = \frac{n!}{i!(n-i)!}$. Since, the structure of such system is a zinc blend structure, therefore n=12 and i varies from 0 to 12. But this does not mean that such method cannot be applied for other structures. The interaction coupling for such distribution ($A\ or\ A'$) is assumed to be:

$$J_{AA'}^i = (J_A^{n-i} J_{A'}^i)^{1/n}. \quad (2.7)$$

Therefore, for the zinc blend structure we can define:-

$$J_{AA'}^i(x) = \sum_{i=0}^{12} K_n^i x^{n-i}(1-x)^i \, (J_A^{n-i} J_{A'}^i)^{1/n}. \quad (2.8)$$

When the interaction couplings $J_A(J_{A'})$ correspond to the nearest neighbor (nn), then $J_{AA'}^i(x) = J_1$. But if $J_A(J_{A'})$ corresponds to the next nearest neighbor (nnn), $J_{AA'}^i(x) = J_2$.

3. HIGH-TEMPERATURE SERIES EXPANSION (HTSE)

In order to expand the magnetic susceptibility by using High- Temperature Series Expansion, first we have to find the relationship between susceptibility and correlation function i.e.

$$\chi(T) = \frac{\beta}{N}\sum_{ij}\langle \boldsymbol{s_i}.\boldsymbol{s_j}\rangle \quad (3.1)$$

By definition specific heat is the first derivative of internal energy with respect to temperature. But here the average energy of the system can be considered as internal energy and magnetic specific heat [12] of the system can be defined as:-

$$C(T) = \frac{d\langle H\rangle}{dT} = \frac{1}{N}\frac{d}{dT}\left(\frac{TrHe^{-\beta H}}{Tre^{-\beta H}}\right) = \frac{1}{N}\frac{d}{dT}\left(\frac{-\frac{d}{d\beta}Tr\{e^{-\beta H}\}}{Tr\{e^{-\beta H}\}}\right). \quad (3.2)$$

From this equation average energy can be defined as:-

$$\langle H\rangle = \frac{TrHe^{-\beta H}}{Tre^{-\beta H}}, \quad (3.3)$$

or

$$\langle H_c \rangle = \frac{\sum_{n=1}^{m} E_n(c) \exp(-\beta E_n(c))}{\sum_{n=1}^{m} \exp(-\beta E_n(c))}. \quad (3.4)$$

Where H_c is the Hamiltonian for the finite cluster c with eigenvalues $E_n(c)$ and m is size of the cluster and the specific heat per site:-

$$c_v = \frac{1}{N} \frac{\langle H^2 \rangle - \langle H \rangle^2}{T^2}. \quad (3.5)$$

Where β is inverse temperature ($\beta = \frac{1}{k_B T}$) and N is the number of magnetic ions. Expression for the correlation function at the sites between i and j would be

$$\langle \boldsymbol{s_i}.\boldsymbol{s_j} \rangle = \frac{Tr S_i S_j exp(-\beta H)}{Trexp(-\beta H)}. \quad (3.6)$$

Expansion of the correlation function in powers of

$$\langle \boldsymbol{s_i}.\boldsymbol{s_j} \rangle = \frac{Tr S_i S_j exp(-\beta H)}{Trexp(-\beta H)} = \sum_{l=0}^{\infty} \frac{(-1)^l}{l!} \alpha_l \beta^l. \quad (3.7)$$

Where $\alpha_l = \nu_l - \sum_{k=0}^{l-1} C_k^l \alpha_k \mu_{l-k}$, $\nu_m = \langle \boldsymbol{s_i}.\boldsymbol{s_j} H^m \rangle$, and $\mu_m = \langle H^m \rangle$.

The calculation of α_l leads to a diagrammatic representation according to [13]. This can be done by using two basic steps:

1. Identifying and cataloguing of all diagrams or graphs which can be constructed from one dashed line connecting the site *i* and *j*, and *l* straight lines, and the determination of diagrams whose contribution is non vanishing. This step has already been accomplished in the Stanley work [14].
2. Counting the number of times that each diagram can occur in the magnetic system. Expansion as power series in reciprocal temperature of the zero-field susceptibility of a magnetic system using correlation function to order six in β can be defined as:-

$$\chi(\beta) = \sum_{m=-n}^{n} \sum_{n=1}^{6} d(m,n) \zeta^m t^n, \quad (3.8)$$

$$\xi^2(\beta) = \sum_{m=-n}^{n} \sum_{n=1}^{6} c(m,n) \zeta^m t^n . \quad (3.9)$$

Where $\zeta = \frac{J_2}{J_1}$ and $= \frac{2S(S+1)J_1}{k_B T}$. Spin glass susceptibility (χ_{SG}) is non linear. This is because of the order parameter (q) is non linear i.e. the self-overlap, also called Edwards-Anderson [15] parameter is defined as

$$q = \frac{1}{N} \sum_i [\langle S_i \rangle^2]_{av} . \quad (3.10)$$

This leads to the magnetic Spin glass susceptibility (χ_{SG}) as

$$\chi_{SG} = \frac{1}{NT^3} \sum_{ij} \left[\langle S_i S_j \rangle^2 \right]_{av}, \quad (3.11)$$

where the correlation length of the correlation function $\left[\langle S_i S_j\rangle^2\right]_{av}$ possibly diverges at $T = T_{SG}$.

4. PADÉ APPROXIMANTS (P.A)

Padé approximants (P.A) [16] have been extensively used for the analysis of high-temperature series expansions [17]. A [L, K] Padé approximants to a function $f(x) = \sum_{i=0}^{N} b_i\, x^i$ is a rational fraction $P_L(x)/Q_K(x)$ where P_L and Q_K are polynomials with degrees L and K respectively. Therefore,

$$f(x) = P_L(x)/Q_K(x) + O(x^{K+L+1}). \tag{4.1}$$

In our case, P.A (L,K) to a series $\chi(T) = \sum_{m=-n}^{n}\sum_{n=1}^{6} d(m,n)\zeta^m t^n$ or $\xi^2(T) = \sum_{m=-n}^{n}\sum_{n=1}^{6} c(m,n)\zeta^m t^n$ is a rational fraction i.e.

$$\chi(T)\ or\ \xi^2(T) \approx\ P_L(x)/Q_K(x) + O(x^{K+L+1}). \tag{4.2}$$

Close to a second-order phase transition at finite temperature T_c^{-1} from a paramagnetic to an ordered state, thermodynamic quantities generally diverge as

$$\chi(T) \propto (T - T_c)^{-\gamma}, \tag{4.3}$$

and

$$\xi^2(T) \propto (T_c - T)^{-2\nu}. \tag{4.4}$$

The Padé approximants to the logarithmic derive ($dln\ \chi(T)/dT \approx \frac{-\gamma}{T-T_c}$) help to determine the critical temperature, the critical exponents of the susceptibility and correlation function $\gamma\ and\ \nu$ respectively.

5. RESULTS AND DISCUSSION

By using mean- field approximation and experimental values for the Neel temperature and the Curie Weiss temperature of the materials, we determined the nearest neighbor (nn) and next nearest neighbor (nnn) exchange interaction couplings for the ordered state. By taking into consideration the disordered state i.e. using probability distribution, we have computed both interaction couplings. The critical exponents associated with magnetic susceptibility and correlation function $\gamma = 1.38 \pm 0.1$ and $\nu = 0.8 \pm o.1$ respectively were also obtained. Based on these exchange coupling and using Padé approximants we presented concentration dependent transition temperature (Phase diagram) as follows:

In this case we can justify that there is spin glass phase in range $(0.2 \leq x < 0.6)$ and antiferromagnetism in range $(0.6 \leq x \leq 1)$ based on exchange interaction coupling calculations. Fig1 explains about different magnetic phases for different concentration regions.

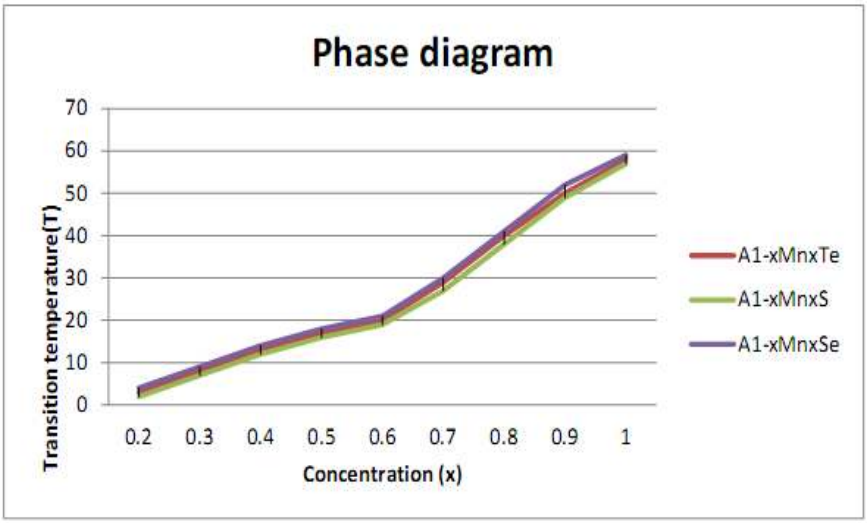

Fig. 1. explains the relationship between the magnetic phase transition temperatures versus magnetic impurity concentration of $A_{1-x}Mn_xA'$

Fig. 2 shows a plot of specific heat(C) vs. temperature for different materials at the same concentration of impurities. As we can see from the figure there is a clear evidence for temperatures getting small the specific heat approaches to zero. The peaks of the curves for these materials are broad which are similar to experimentally observed ones. Obviously, when the temperature is reduced, the value of thermal fluctuations become small and the C will also be small. At high temperature the specific heat tends to constant value as all microstates are equally occupied. However, the fluctuations of the energy are approaching maximum value near $^{T}/_{J} \sim 0.6$, giving a specific heat peak.

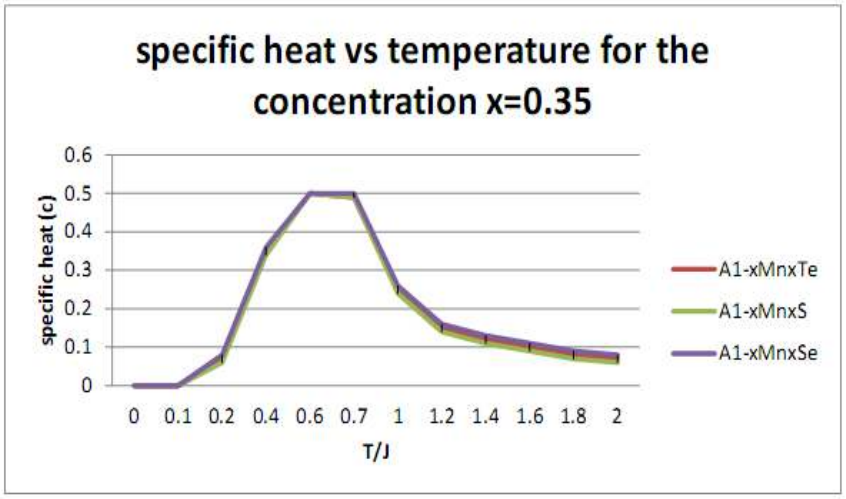

Fig. 2. Schematic representation of magnetic specific heat (J/mole k) vs. temperature (k) for the materials ($A_{1-x}Mn_xA'$)

6. CONCLUSIONS

In the present work the exchange integrals (J_1 and J_2) for nearest neighbor (nn) and next nearest neighbor interactions (nnn) using mean-field approximation in concentration range ($0.6 \leq x \leq 1$) and taking into consideration the dilution problem we used probability distribution in range ($0.2 \leq x < 0.6$) for the systems were computed. We used these values for magnetic susceptibility and magnetic specific heat calculations. In order to determine the susceptibility and specific heat, we employed high temperature series expansion and Pad*é* approximants at the critical region. Different magnetic phases such as (spin glass, antiferromagnetic and paramagnetic) based on their concentration ranges were established and the findings are in agreement with previous studies.

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COMPETING INTERESTS

Authors have declared that no competing interests exist.

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