Effects of a Magnetic Field on the Thermodynamics of Dilute Classical Spin Chains

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EFFECTS OF A MAGNETIC FIELD ON THE THERMODYNAMICS
OF DILUTE CLASSICAL SPIN CHAINS

by

Guoqing Hu

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EFFECTS OF A MAGNETIC FIELD ON THE THERMODYNAMICS
OF DILUTE CLASSICAL SPIN CHAINS

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Western Michigan University, 1987

The thermodynamics of a diluted chain of ferromagnetic classical spin in the presence of an external magnetic field is determined in the limit of the continuum model. The magnetization, susceptibility, specific heat are determined for both the isotropic Heisenberg and the classical XY models as functions of temperature, magnetic field and magnetic concentration. Scaling law for the behavior of the thermodynamic quantities in field, temperature, and magnetic concentration are obtained.

The calculations will be based on the continuum model of classical spin which was solved for the infinite chain system by McGurn and Scalapino.
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Guoqing Hu
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# TABLE OF CONTENTS

ACKNOWLEDGEMENTS ....................................................... ii  
LIST OF FIGURES ....................................................... iv  

CHAPTER  

I. INTRODUCTION ......................................................... 1  
II. ISOTROPIC HEISENBERG CHAIN ........................................ 4  
   The Theory ......................................................... 4  
   The Results ....................................................... 7  
III. CLASSICAL XY MODEL ............................................... 15  
   The Theory ......................................................... 15  
   The Results ....................................................... 17  
IV. CONCLUSION .......................................................... 23  

APPENDIX  

   Standard Techniques .................................................. 24  

BIBLIOGRAPHY ............................................................ 27
LIST OF FIGURES

1. Magnetization per Site Versus $kT/\sqrt{2Jh}$ ........................................ 11
2. Magnetization per Site Versus $\sqrt{N/2J}$ ........................................ 12
3. $(kT/g\beta^2)\sqrt{N/2J}X$ Versus $kT/\sqrt{2Jh}$ ................................ 13
4. $(\Delta C/k)\sqrt{2Jh}$ Versus $kT/\sqrt{2Jh}$ ........................................ 14
5. Magnetization per Site Versus $kT/\sqrt{2Jh}$ for the Pure System Infinite Chain XY Model ........................................ 20
6. Magnetization per Site Versus $kT/\sqrt{2Jh}$ .................................... 21
7. Susceptibility, $\chi$, Versus $kT/\sqrt{2Jh}$ ......................................... 22
CHAPTER I

INTRODUCTION

Magnetic materials in which the molecular geometry is such that the exchange coupling between spins along a certain one-dimensional chain is much larger than the coupling between the chains, these systems can be described in terms of one-dimensional models. One-dimensional models have long been of theoretical interest, largely because of the relative ease in structing models that can be actually solved in some cases exactly. Especially on account of the discovery of real magnets whose properties closely approximate those one-dimensional models, in recent years, these models have been widely studied\textsuperscript{1-11}.

Some one-dimensional models, like, the Heisenberg, the XY and the Ising models are particularly of theoretical interest, because magnetic interactions are more simplified. The definitions of these models are as follows: the interaction Hamiltonian

\[ \mathcal{H} = -2J \sum_{i>j} [a S_i^x S_j^x + b (S_i^y S_j^y + S_i^z S_j^z)] \]  \text{(1.1)}

where summation is taken over nearest neighboring spins and $J$ is the exchange constant. When $a=1$ and $b=1$, it gives the Heisenberg model, in which the interaction is wholly isotropic. The anisotropic Ising model, is obtained by setting $a=1$ and $b=0$. the case $a=0$ and $b=1$ is called the XY model. The pure magnetic materials do not really exist, there are always some impurities in them. In some cases these impurities are nonmagnetic so that they breakup the chain into isolated chain segments of finite lengths. These systems are called diluted systems.
From a theoretical standpoint solutions have been obtained for the diluted XY quantum chain with\textsuperscript{8} and without\textsuperscript{11} an external applied magnetic field, for the diluted Ising system, for the spin-wave approximation to the low-temperature limit of the quantum system\textsuperscript{6,9}, and for the isotropic Heisenberg chain of classical spin in the absence of external magnetic fields\textsuperscript{10}. These solutions are obtained by first solving for the properties of chains of finite lengths and then obtaining the diluted system results as a weighted sum over the finite chain results.

Unfortunately, the only realistic quantum model which has been solved for finite chains is the XY model so that most of the above work is confined to classical models and to the spin-wave approximation. But classical Heisenberg model has been successful in describing a number of properties, though, for a system in the absent of an external field. In this paper, the work is made to obtain properties of classical systems within an external field. These systems have not been studied previously.

By comparison of theoretical results with experimental results, classical spin systems have been found to yield useful approximations for the properties of infinite and long chains of spin, but fail for small chains where the discrete nature of the energy levels of the quantum chains are badly given in the classical system.

But diluted solutions of classical models are still of interest. First, they give good representations of small dilution systems, and second, by experimental comparison allowing for the determination of the regions of validity of these models and offering insight into the modifications necessary to correctly describe experimental results.

In this paper the thermodynamics for a diluted chain of classical spin in the presence of an external magnetic field is determined. The
calculations will be based on the continuum model of classical spin which was solved for the infinite chain system by McGurn and Scalapino (1975). This model gives a successful representation of the classical system for regions of long spin-spin correlation lengths. The field-dependent magnetizations, susceptibility and specific heat are determined for both the isotropic Heisenberg and classical XY models as functions of temperature, field and magnetic concentration.
CHAPTER II

ISOTROPIC HEISENBERG CHAIN

The Theory

In a one-dimensional diluted Heisenberg chain system, the exchange coupling between nearest neighboring spins is much stronger than the other interactions, then, one can ignore dipole-dipole interactions within and between the finite segments, treating the properties of each segments as being independent of the other finite segments in the system, and in addition assuming that the nonmagnetic impurities occur randomly and have no correlations between them, the partition function of such a dilute system is written as a product of the partition function of the individual chains that occur in the system.

\[
Z(T, H, p) = \prod_{L=1}^{\infty} \left[ Z_L(T, H) \right]^{N(1-p)^2 p^L},
\]

where \( p \) is the concentration of spins present in the system of \( N \to \infty \) lattice sites, the concentration of nonmagnetic impurities is \( (1-p) \), the number of \( L \) spins chain is then \( N(1-p)^2 p^L \), and \( Z_L(T, H) \) is the partition function for a chain of \( L \) spins. The magnetization and specific heat per lattice site of the diluted system are obtained from appropriate derivates of the logarithm of the partition function\(^6,8,9,11\). It follows:

\[
M(T, H, p) = (1-p)^2 \sum_{L=1}^{\infty} M_L(T, H) \cdot p^L,
\]

and

\[
C(T, H, p) = (1-p)^2 \sum_{L=1}^{\infty} C_L(T, H) \cdot p^L.
\]
where $M_L(T,H)$ and $C_L(T,H)$ are the magnetic moment and specific heat of a chain of $L$ spins. The magnetic susceptibility parallel to the field is easily obtained by taking appropriate derivative of the magnetization:

$$\chi(T,H,p) = (1-p) \sum_{L=1}^{\infty} \chi_L(T,H) p^L.$$  \hspace{0.5cm} (2.4)

The Hamiltonian of the diluted chain of classical spins is given by

$$H_0 = -\sum_{i=1}^{L} 2J \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} - g \mu H \sum_{i=1}^{L} S_i^z.$$  \hspace{0.5cm} (2.5)

Here $\{\boldsymbol{S}_i\}$ are classical unit vectors at the discrete sites of the lattice and $C_i = 1$ or 0 dependent on whether or not a spin is present on the $i$th site.

The function $M_L(T,H)$ and $C_L(T,H)$ for chains of $L$ spins can be obtained by considering the $L$-spins Hamiltonian

$$H_L = -\sum_{i=1}^{L} 2J \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} - g \mu H \sum_{i=1}^{L} S_i^z.$$  \hspace{0.5cm} (2.6)

In the low-temperature region, $2J/kT > 1$, the system in Eq. (2.6) can be approximated by the continuum model limit with Hamiltonian

$$\mathcal{G}_L \left[ \tilde{S}(x) \right] = \int_0^L dx \left[ J \left| \frac{d\tilde{S}(x)}{dx} \right|^2 - h \tilde{S}^z(x) \right].$$  \hspace{0.5cm} (2.7)

where $h = g \mu H$ and $\tilde{S}(x)$ is a unit vector at point $x$.

The partition function for a chain of lengths $L$ in the continuum model is then given by:

$$Z_L = \int \delta \tilde{S}(x) e^{-\beta \mathcal{G}_L \left[ \tilde{S}(x) \right]}.$$  \hspace{0.5cm} (2.8)

where $\beta = 1/kT$. By using standard techniques (see appendix), one finds

$$Z_L = \sum_{n=0}^{\infty} |a_n|^2 e^{-\beta E_n},$$  \hspace{0.5cm} (2.9a)
with
\[ A_n = \int d\theta d\phi \phi_n(\theta, \phi), \]
\[ E_n = E_0 + \varepsilon_n, \]
where \( \phi_n(\theta, \phi) \) and \( \varepsilon_n \) satisfy the eigenvalue equation
\[ \left[ \frac{\mathcal{L}^2}{4\beta^2} - h\cos\theta \right] \phi_n(\theta, \phi) = \varepsilon_n \phi_n(\theta, \phi) \]
(2.10)
\( (n=0,1,2,\ldots) \) for states of no \( \theta \) dependence, with
\[ \mathcal{L}^2 = -\frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \left( \sin\theta \frac{\partial}{\partial \theta} \right) - \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial \phi^2} \]
(2.11)
and \( E_0 = kT \ln (\beta2J) \) is a constant independent of \( n \).

In order to obtain the expression of the magnetization of the chain, the additional functional integral
\[ N_L(x_i) = \int d^3 \tilde{z}(x) \tilde{z}(x_i) e^{-\beta \mathcal{L}_L \tilde{z}(x)} \]
(2.12)
is needed to evaluate. Applying standard techniques (see appendix) to \( N_L(x_i) \) yields
\[ N_L(x_i) = \sum_{n,m} a_n\alpha_m^* \langle n|\cos\theta|m \rangle \cdot e^{-\beta \Phi_1(E_n - E_m)} e^{-\beta E_m L} \]
(2.13)
where using Dirac notation
\[ \langle n|\cos\theta|m \rangle = \int d\theta d\phi \phi_n^*(\theta, \phi) \cos\theta \phi_m(\theta, \phi). \]
(2.14)
The total magnetic moment of the chain of length \( L \) is then
\[ M_L(T, H) = \int_0^L dx_i \frac{N_L(x_i)}{Z_L} \]
\[ = \left[ \sum_n \sum_{m \neq n} a_n \alpha_m^* \frac{\langle n|\cos\theta|m \rangle}{\beta(E_m - E_n)} \left( e^{-\beta E_n} - e^{-\beta E_m} \right) \right. \]
\[ + L \sum_n |a_n|^2 \langle n|\cos\theta|n \rangle e^{-\beta E_n} \int \left[ \sum_n |a_n|^2 e^{\beta E_n} \right] \]
(2.15)
and the susceptibility is

\[ \chi_c(T, H) = \frac{2}{\beta H} M_c(T, H). \]  \hspace{1cm} (2.16)

In obtaining these results, it is needed to evaluate Eq. (2.10), multiplying \( \sqrt{2J} / \hbar \beta \) to both sides of Eq. (2.10), it gives

\[ \sqrt{2J} / \hbar \beta \left[ \frac{d^2}{d\theta^2} - \hbar \cos \theta \right] \phi_n(\theta, \varphi) = \sqrt{2J} / \hbar \beta \epsilon_n \phi_n(\theta, \varphi), \]  \hspace{1cm} (2.17)

leads to

\[ \left[ \frac{d^2}{d\theta^2} - \sqrt{2J} / \hbar \beta \cos \theta \right] \phi_n(\theta, \varphi) = \sqrt{2J} / \hbar \beta \epsilon_n \phi_n(\theta, \varphi), \]  \hspace{1cm} (2.18)

same as

\[ \left[ \frac{d^2}{d\theta^2} - \chi \cos \theta \right] \phi_n(\theta, \varphi) = \lambda_n \phi_n(\theta, \varphi), \]  \hspace{1cm} (2.19)

where \( \chi = \sqrt{2J} / \hbar \beta \), \( \lambda_n = \epsilon_n \sqrt{2J} / \hbar \beta \).

By using Hamiltonian matrix techniques, it gives

\[ H_{ll'} = \langle l'0 | \frac{d^2}{d\theta^2} - \chi \cos \theta | l'o \rangle = \frac{1}{2 \lambda} \delta_{ll'} - \chi \sqrt{\frac{\lambda}{3}} \langle l'0 | l'o \rangle, \]  \hspace{1cm} (2.20)

where \( \langle l'0 | l'o \rangle \) is just the Clebsch-Gordan coefficient. Since the Hamiltonian matrix is formed, it is easy to solve for the eigenvalue and eigenvector which are only dependent on \( kT / \sqrt{2J} \hbar \) and \( \sqrt{\hbar / 2J} \). Here 25x25 matrix are used to be solved on computer, which gives good approximation value for these results.

The Results

The results of the thermodynamical properties of these systems can be obtained in the large field, \( h >> J \), limit, for fixed values of \( kT / \sqrt{2J} \hbar \) and
In the limit $\sqrt{\frac{H}{2J}} \to \infty$, which leads to $a_n = 0$ ($n \neq 0$), $a_0 = 1$, and one finds that Eq. (2.15) gives:

$$M_L(T, H, p) = L \langle 0| \cos \theta | 0 \rangle,$$

(2.21)

where $\langle 0| \cos \theta | 0 \rangle$ depends only on $kT/\sqrt{2JH}$ and is just the magnetization per lattice site of the infinite-chain. Using Eqs. (2.21) and (2.2), the magnetization per lattice site of the dilute system is then given by

$$M(T, H, p) = p \langle 0| \cos \theta | 0 \rangle,$$

(2.22)

while for small fields the magnetization always falls away from that of Eq. (2.22). In the large field limit, one finds from Eq. (2.22) that the normalized susceptibility of the diluted system is given by

$$\frac{kT}{g^2u} \left[ \frac{h}{2T} \right]^\frac{3}{2} \chi = p \frac{kT}{g^2u} \left[ \frac{h}{2T} \right]^\frac{3}{2} \chi_{\infty}(kT/\sqrt{2JH}),$$

(2.23)

where $\chi_{\infty}$ is the infinite-chain result. It is interesting that in this large field limit one finds that the magnetization and, consequently, the normalized susceptibility of Eq. (2.23), as in the pure system, only depend on one reduced parameter, i.e., $kT/\sqrt{2JH}$. This dependence for pure system properties has been found experimentally.

In Figs. 1(a)-1(d), the general field magnetization from Eqs. (2.2) and (2.15) versus $kT/\sqrt{2JH}$ for concentrations $p = 0.9, 0.8, 0.7, \text{ and } 0.5$ are plotted. Curves for $\sqrt{\frac{H}{2J}} = 0.1, 0.5, \text{ and } 1.0$ are presented. For these plots, $M_L(T,H)$ for $L>1$ are given by Eq. (2.15) and

$$M_L(T, H) = \coth \left( \frac{H}{L} \right) - \frac{1}{LH},$$

(2.24)

which is the result for a single paramagnetic spin in an external field.

One finds that as $\sqrt{\frac{H}{2J}}$ becomes larger than 1.0, for a fixed $kT/\sqrt{2JH}$
and for \( p > 0.6 \), the curves in Fig. 1 saturate at the results in Eq.(2.22), but for smaller fields the deviation from this saturation value can be quite significant. In Figs.(2a) and (2b), \( M(T,H,p) \) versus \( \sqrt{h/2J} \) for fixed \( p=0.9 \) and 0.7 and fixed values of \( kT/\sqrt{2Jh} \) are plotted. These plots display the rapidity at which saturation in the field is achieved for \( \sqrt{h/2J} > 1.0 \) at a given \( kT/\sqrt{2Jh} \) value. It should be noted in these plots that the curves which differ significantly from the saturation curves do not obey any simple scaling laws in \( J, h, T, \) or \( p \).

In Figs. 3(a)-3(b), the susceptibility versus \( kT/\sqrt{2Jh} \) for values of \( \sqrt{h/2J} = 0.1, 0.5, \) and 1.0 are plotted. These curves are easily obtained from the derivatives of the curves plotted in Figure1. Again a significant dependence of the susceptibility on \( \sqrt{h/2J} < 1 \) is seen for a fixed \( kT/\sqrt{2Jh} \).

The specific heat of this system can be written from Eqs(2.3) and (2.8) as

\[
C(T, H, p) = p C_{\infty} + \Delta C(T, H, p),
\]

(2.25)

where \( C_{\infty} \) is the specific heat per lattice site of an infinite chain in an external magnetic field, \( H, \) and \( \Delta C(T, H, p) \) is the correction to the \( pC_{\infty} \) term. From Eqs. (2.8)-(2.14) it gives

\[
\Delta C(T, H, p) = (1-p)^3 \sum_{L=1}^{\infty} p^{L} \frac{\partial}{\partial p} \frac{\partial^{L}}{\partial p^{L}} \ln \left[ \sum_{n \geq 0} |a_n|^2 e^{-p \varepsilon_n} \right].
\]

(2.26)

Again fixing \( kT/\sqrt{2Jh} \) and taking the limit of Eq(2.22) as \( \sqrt{2Jh} \to \infty \) one finds

\[
\Delta C(T, H, p) \to 2 p (1-p) \frac{\partial}{\partial p} \ln |a_0|.
\]

(2.27)

In Figs. 4(a) and 4(b), \( (\Delta C/k)/\sqrt{2Jh} \) versus \( kT/\sqrt{2Jh} \) for magnetic
concentrations $p=0.9$ and $0.7$ are plotted. Curves for $\sqrt{2J}=0.1$ and 0.5 are presented. The corrections to the $pC_\infty$ first term in Eq. (2.25) are seen to be very small.
Figure 1. Magnetization per Site Versus $kT/\sqrt{2}J_h$ for $\sqrt{J/2J} = 0.1$ (Dash-Dotted Line), 0.5 (Solid Line), and 1.0 (Dashed Line) for (a) $p=0.9$, (b) $p=0.8$, (c) $p=0.7$, and (d) $p=0.5$. (Note: For the pure system the saturation magnetization per site is $M=1.0$)
Figure 2. Plot of the Magnetization per Site Versus $\sqrt{\frac{\hbar}{2J}}$ for $kT/\sqrt{2J} = 0.5$ (Dashed-Dotted Line), 1.0 (Solid Line), and 2.0 (Dashed Line) for (a) $p=0.9$ and (b) $p=0.7$. (The asymptotic limits of the curves in the limit that $\sqrt{\frac{\hbar}{2J}} \to \infty$ are indicated by horizontal lines on the right-hand side of these figures.)
Figure 3. Plots of \((kT/g^2 \xi^2)^{\sqrt{h/2J}} Z\) Versus \(kT/\sqrt{2Jh}\) for \(\sqrt{h/2J} = 0.1\) (Dashed-Dotted Line), 0.5 (Solid Line), and 1.0 (Dashed Line) for (a) \(p=0.9\), (b) \(p=0.8\), (c) \(p=0.7\), and (d) \(p=0.5\).
Figure 4. Plots of $\frac{AC/k}{\sqrt{2J/h}}$ versus $kT/\sqrt{2Jh}$ for $\sqrt{h/2J} = 0.1$ (Dashed-Dotted Line) and 0.5 (Solid Line) for (a) $p=0.9$ and (b) $p=0.7$. 

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CHAPTER III

Classical XY Model

The Theory

Almost same as in chapter II, in order to obtain the expressions of the properties of the classical XY chain, it is needed to evaluate the partition function of classical XY chain first. The Hamiltonian of the diluted XY chain of classical spins is given by

\[ H_o = -\sum_{i} 2J \mathbf{s}_i \cdot \mathbf{s}_{i+1} - g\mu H \sum_{i} \mathbf{s}_i^x. \]  \hspace{1cm} (3.1)

Here \( \mathbf{s}_i \) are classical unit vectors confined to be in the X-Y plane, \( c_i = 1 \) or 0 dependent on whether or not a spin is present on the \( i \)th site, and the external magnetic field, \( H \), is taken along the x axis. This leads to that the Hamiltonian of \( L \) spins XY chain is given by

\[ H_L = -\sum_{i=1}^{L} 2J \mathbf{s}_i \cdot \mathbf{s}_{i+1} - g\mu H \sum_{i=1}^{L} \mathbf{s}_i^x. \]  \hspace{1cm} (3.2)

Same as before, in the limit that \( 2J/kT > 1 \), Eq. (3.2) by the continuum limit becomes

\[ \mathcal{H}_L[\mathbf{S}(x)] = \int_0^L dx \left[ J \left| \frac{d\mathbf{S}(x)}{dx} \right|^2 - h \mathbf{S}^x(x) \right]. \]  \hspace{1cm} (3.3)

Here \( h=g\mu H \) and \( \mathbf{S}(x)=\mathbf{n}(x) \), with \( \mathbf{n}(x) \) being a unit vector in the X-Y plane at point \( x \) on the chain.

It follows that the partition function for a chain of length \( L \) is given in the continuum limit by

\[ Z_L = \int \mathcal{D}[\mathbf{S}(x)] \ e^{-\int \mathcal{H}_L[\mathbf{S}(x)]}. \]  \hspace{1cm} (3.4)
By using standard techniques \(^4,7\) (see appendix), this can be evaluated to yield

\[
Z_L = \sum_{n=-\infty}^{\infty} |a_n|^2 e^{-\beta \xi n}
\]

(3.5)

with

\[
\begin{align*}
\alpha_n &= \int_0^{2\pi} d\theta \, \phi_n(\theta), \\
E_n &= E_0 + \xi n.
\end{align*}
\]

(3.6) (3.7)

where \(\phi_n(\theta)\) and \(\xi n\) satisfy the eigenvalue equation

\[
- \left[ \frac{\partial^2}{\partial \theta^2} + h \cos \theta \right] \phi_n(\theta) = \beta \xi n \phi_n(\theta) \quad (n = 0, \pm 1, \pm 2, \ldots)
\]

(3.8)

and \(E_0\) is a constant independent of \(n\).

To obtain the magnetization of the chain, it is necessary to evaluate

\[
N_L(x_i) = \langle s^x(X) s^x(X_0) e^{-\beta \xi [s^x(V_m)]} \rangle
\]

\[
= \sum_n a_n^* a_n \langle n | \cos \theta | m \rangle e^{-\beta \xi (E_n - E_m)} e^{-\beta \xi E_m}
\]

(3.9)

where

\[
\langle n | \cos \theta | m \rangle = \int \frac{d\theta}{2\pi} \phi_n^*(\theta) \cos(\theta) \phi_m(\theta)
\]

(3.10)

Then

\[
M_L(T, H) = \frac{1}{Z_L} \int_0^L dx_i N_L(x_i)
\]

\[
= \left[ \sum_n a_n^* a_n \langle n | \cos \theta | m \rangle (e^{-\beta \xi E_n} - e^{-\beta \xi E_m}) \right] + L \sum_n |a_n|^2 \langle n | \cos \theta | n \rangle e^{-\beta \xi E_n} / \sum_n |a_n|^2 e^{-\beta \xi E_n}
\]

(3.11)

and the susceptibility is given by

\[
\chi_L(T, H) = \frac{\partial}{\partial H} M_L(T, H).
\]

(3.12)
In obtaining these results, it is needed to evaluate Eq. (3.8),
multiplying $\sqrt{2J/\hbar \beta}$ to both sides of Eq. (3.8), it gives

$$-\sqrt{2J/\hbar \beta} \left[ \frac{1}{4\beta} \frac{\partial^2}{\partial \theta^2} + \hbar \cos \theta \right] \phi_n(\theta) = \sqrt{2J/\hbar \beta} \epsilon_n \phi_n(\theta),$$

(3.13)

leads to

$$-\left[ \frac{1}{2\sqrt{2J/\hbar \beta}} \frac{\partial^2}{\partial \theta^2} + \sqrt{2J/\hbar \beta} \cos \theta \right] \phi_n(\theta) = \sqrt{2J/\hbar \beta} \epsilon_n \phi_n(\theta),$$

(3.14)

same as

$$-\left[ \frac{1}{2x'} \frac{\partial^2}{\partial \theta^2} + x' \cos \theta \right] \phi_n(\theta) = \lambda_n \phi_n(\theta),$$

(3.15)

where $x' = \sqrt{2J/\hbar \beta}, \lambda_n = \sqrt{2J/\hbar \beta}$.

Using Hamiltonian matrix techniques, it gives

$$H_{LL'} = \langle \ell | - \frac{1}{2x'} \frac{\partial^2}{\partial \theta^2} - x' \cos \theta | \ell' \rangle$$

$$= - \frac{\delta \epsilon'}{2x'} \delta_{LL'} - x' \langle \ell | \cos \theta | \ell' \rangle,$$

$$\langle \ell | \cos \theta | \ell' \rangle = \int \cos(\ell \theta) \cos \theta \cos(\ell' \theta) d\theta$$

$$= \begin{cases} 1 & \ell = \pm \ell' + 1 \\ 0 & \ell \neq \pm \ell' + 1 \end{cases}$$

(3.16)

Since the Hamiltonian matrix is formed, it is easy to solve for the eigenvalue and eigenvector which are only dependent on $kT/\sqrt{2J}$ and $\sqrt{h/2J}$. Here 25x25 matrix are used to be solved on computer, which gives good approximation value for these results.

The Results

The results for the diluted system can be obtained by using Eqs. (3.11) and (3.12) in Eqs. (2.2) and (2.4). The infinite chain magnetization and susceptibility are given by
\[ M_{\infty}(T, H) = \langle 0 | \cos \phi | 0 \rangle \]  
(3.17)

where \( \langle 0 | \cos \phi | 0 \rangle \) depends only on \( kT/\sqrt{2Jh} \) and

\[ \chi_{\infty} = g \mu_B \frac{2}{kT} M_{\infty}(T, H). \]  
(3.18)

These two results are plotted in Figs. 5(a) and 5(b), respectively. 

From Eqs. (3.11) and (3.12), one finds for a fixed value of \( kT/\sqrt{2Jh} \), the \( \sqrt{2J}/\lambda \to \infty \) limit gives

\[ M_L(T, H) = L M_{\infty}(T, H), \]  
(3.19)

and a similar limit for \( \chi_L(T, H) \). Hence for the diluted system in this limit one finds

\[ M(T, H, p) \to P M_{\infty}(T, H), \]  
(3.20a)

\[ \chi(T, H, p) \to \chi_{\infty}(T, H). \]  
(3.20b)

In Figs. 6(a)-6(d), \( M(T, H, p) \) versus \( kT/\sqrt{2Jh} \) for magnetic concentration \( p=0.9, 0.8, 0.7, \) and 0.5 are plotted. Curves for \( \sqrt{2J}/\lambda =0.1, 0.5, 1.0, \) and 5.0 are presented. For these curves, \( M_L(T, H) \) for \( L>1 \) to be given by Eq. (3.11) and

\[ M_l(T, H) = I_1(\beta H)/I_0(\beta H). \]  
(3.21)

which is the results for a single paramagnetic XY spin in an external magnetic field. The corresponding curves for the susceptibility are obtained by taking the derivative of the curves in Fig 6. The susceptibility is plotted in Figs. 7(a)-7(d).

From Eqs. (3.20a), and (3.21) one finds that in the large \( \sqrt{2J}/\lambda \) limit for \( p>0.6 \), the scaling relations in \( kT/\sqrt{2Jh} \) for \( M \) and \( \sqrt{2J}/\lambda \chi \) are similar to those obtained for the isotropic Heisenberg system, i.e.,
\[ M = \rho M_\infty \left( \frac{KT}{\sqrt{2Jh}} \right), \]

\[ \left[ \frac{h}{2J} \right]^\frac{1}{2} \mathcal{X} = \rho \left[ \frac{h}{2J} \right]^\frac{1}{2} \mathcal{X}_\infty \left( \frac{KT}{\sqrt{2Jh}} \right). \] (3.22a)

(3.22b)
Figure 5. (a) Magnetization per Site Versus $kT/2Jh$ for the Pure System Infinite Chain XY Model. (b) Susceptibility Parallel to the Field, $\chi$, Versus $kT/2Jh$ for the Infinite Chain XY Model.
Figure 6. Magnetization per Site Versus $kT/\sqrt{Jh}$ for $\sqrt{Jh}/2J = 0.1$ (Dashed-Dotted Line), 0.5 (Solid Line), 1.0 (Dashed Line), and 5.0 (Solid-Dashed Line) for (a) $p = 0.9$, (b) $p = 0.8$, (c) $p = 0.7$, and (d) $p = 0.5$. 

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Figure 7. Susceptibility $\chi$ versus $kT/\sqrt{2J}$ for $\sqrt{2J}=0.1$ (Dashed-Dotted Line), 0.5 (Solid Line), 1.0 (Dashed Line), and 5.0 (Solid-Dashed Line) for (a) $p=0.9$, (b) $p=0.8$, (c) $p=0.7$, and (d) $p=0.5$. 

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CHAPTER IV

CONCLUSION

In this paper, the thermodynamics of properties of the diluted isotropic Heisenberg and XY classical spin models are calculated in the low-temperature region, \( J/kT > 1 \), which makes it possible to use the continuum limit model of Hamiltonian of the classical chain, and also the nearest neighboring interaction approximation is used to simplify the partition function of the diluted classical chain. By using standard techniques, the problems of solving the thermodynamics of properties of the diluted classical chain becomes the problems of solving the eigenvalue equations which are solved on computer by using Hamiltonian matrix techniques.

The magnetization, susceptibility and specific heat of the diluted systems have been determined as function of the variables \( kT/\sqrt{2Jh} \) and \( \sqrt{h/2J} \). In the large field, \( \sqrt{h/2J} > 1 \), limit and \( p > 0.6 \), the system magnetization and susceptibility are approximately those of the pure system multiplied by the magnetic concentration. These results agree with the experimental results quite well.

It is indicated by this paper that the classical models are not only good for the system in the absence of an external field, but also good for a system with few nonmagnetic impurities within a large external field at low-temperature region.
APPENDIX
Standard Techniques

24
STANDARD TECHNIQUES

To prove

\[ Z_L = \int d\xi(x) e^{-\beta \mathcal{G}[\tilde{\xi}(x)]] = \sum_{n}^{} |a_n|^2 e^{-\beta E_n} } \]

starting from Eqs. (2.7) and (2.8), it follows that:

\[ Z_L = \int d\xi(x) e^{-\beta \mathcal{L} \int d\xi [ J \left( \frac{d\xi}{dx} \right)^2 - h \xi^2(x) ]} \]

This can be written in Riemann form:

\[ Z_L = \int \prod_{j} d\xi_j e^{-\beta \mathcal{L} \int d\xi \left[ J \left( \frac{d\xi}{dx} \right)^2 - h \xi(x) \right]} \]

where

\[ e^{-\beta \mathcal{L} \int d\xi \left[ J \left( \frac{d\xi}{dx} \right)^2 - h \xi(x) \right]} = \sum_{n}^{} \phi_n(\xi(x)) \]

which leads to

\[ e^{-\beta \mathcal{L} \int d\xi \left[ J \left( \frac{d\xi}{dx} \right)^2 - h \xi(x) \right]} \phi_n(\xi(x)) = e^{-\beta E_n \int d\xi} \phi_n(\xi(x)) \]

(A1)

By expanding \( \tilde{\xi}_i \) about \( \tilde{\xi}_{i+1} \) as \( \Delta x \to 0 \) and substituting Eq.(A1) into
Eq. (2.10), gives Eq. (2.9a).

To prove

\[ N_L = \int \delta \tilde{s}^{(x)}(\tilde{z}) e^{-\beta \int \delta \tilde{s}^{(x)}(\tilde{z})} = \sum_{nm} a_n a_m^{*} \left< n | \cos \phi | m \right> e^{\beta \int \left( E_n - E_m \right) e^{-\beta L}} \]

starting from Eqs. (2.7) and (2.12), it follows that:

\[ N_L = \int \delta \tilde{s}^{(x)} \leq \tilde{z}^{(x)} \left[ \int \left( \frac{d\tilde{z}}{dx} \right)^2 - h \tilde{z} \right] \]

This can be written in Riemann form:

\[ N_L = \int \frac{d\tilde{z}}{\delta} \leq \tilde{z}^{(x)} \left[ \int \left( \frac{d\tilde{z}}{dx} \right)^2 - h \tilde{z} \right] \]

\[ = \int \frac{d\tilde{z}}{\delta} \leq \tilde{z}^{(x)} \left[ \int \left( \frac{d\tilde{z}}{dx} \right)^2 - h \tilde{z} \right] \]

where

\[ e^{\beta \int \left( \frac{d\tilde{z}}{dx} \right)^2 - h \tilde{z}} = \sum_{n} \phi_n (\tilde{z}) \]

\[ \phi_n (\tilde{z}) = e^{-\beta E_n \tilde{z}} \]

which leads to

\[ e^{\beta \int \left( \frac{d\tilde{z}}{dx} \right)^2 - h \tilde{z}} \phi_n (\tilde{z}) \]

\[ = e^{-\beta E_n \tilde{z}} \phi_n (\tilde{z}) \]

(A2)

By expanding \( \tilde{z} \) about \( \tilde{z}_{i+1} \) as \( \delta x \rightarrow 0 \) and substituting Eq. (A2) into Eq. (2.10), gives Eq. (2.13).
BIBLIOGRAPHY


