Experimental study of bound magnons and spin cluster resonances in one-dimensional S=1/2, Ising-Heisenberg ferromagnets
by Kathirgamathamby Ravindran

A thesis submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy in Physics
Montana State University

Abstract:
Differential magnetic susceptibility of one-dimensional S=l/2, ferromagnetic compounds, [(CH3)3NH]FeCl3.2H20 (FeTAC), (CH3)4NCuCl3 (TMCuC), and CuCl2C2H6SO (CuCl2.DMSO) are presented. The data are analyzed using the Johnson and Bonner theory to look for expected bound magnon effects. It is found that in FeTAC (Ising) and TMCuC (Heisenberg) the low temperature susceptibility is almost entirely represented by bound state excitations and that the usual spin wave excitations fail to represent the data. Analysis on CuCl2 DMSO shows that owing to the strong interchain exchange significant deviation from a 1-D system occurs below 13K so that the bound magnon effect cannot be clearly identified. It is found that Takahashi’s, and Schlottmann’s recent low temperature expansions for the isotropic Heisenberg ferromagnet fit the zero field data of TMCuC. Numerical results of finite chain calculations of 12-spin, and 14-spin for the isotropic Heisenberg ferromagnet are discussed.

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Date 24 May 1991.

to my mother and late father

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ABSTRACT

Differential magnetic susceptibility of one-dimensional S=1/2, ferromagnetic compounds, $[(CH_3)_3NH]FeCl_3.2H_2O$ (FeTAC), $(CH_3)_4NCuCl_3$ (TMCuC), and $CuCl_2.C_2H_6SO$ ($CuCl_2$.DMSO) are presented. The data are analyzed using the Johnson and Bonner theory to look for expected bound magnon effects. It is found that in FeTAC (Ising) and TMCuC (Heisenberg) the low temperature susceptibility is almost entirely represented by bound state excitations and that the usual spin wave excitations fail to represent the data. Analysis on $CuCl_2$.DMSO shows that owing to the strong interchain exchange significant deviation from a 1-D system occurs below 13K so that the bound magnon effect cannot be clearly identified. It is found that Takahashi's, and Schlottmann's recent low temperature expansions for the isotropic Heisenberg ferromagnet fit the zero field data of TMCuC. Numerical results of finite chain calculations of 12-spin, and 14-spin for the isotropic Heisenberg ferromagnet are discussed.

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CHAPTER 1

INTRODUCTION

The study of thermodynamic properties of magnetic materials has been an excellent way of characterizing them and has lead to a fundamental understanding of their behavior. In recent years a considerable amount of interest has been focussed on trying to understand one-dimensional magnetic systems. It has been shown that there is no long range ordering in one-dimensional magnets except possibly at T=0.[1] Because of the absence of long range ordering the mean field and standard linear spin wave type calculations, which explain three-dimensional magnetic systems, are inadequate for explaining the thermodynamics of the one dimensional case. From the theoretical point of view, these systems are among the simplest non-trivial many-body systems, displaying a large variety of unexpected features resulting from the strong fluctuations.[2] Mikeska demonstrated that an easy plane chain of classical spins (S > 1/2) in a magnetic field can be mapped to a sine-Gordon (SG) equation.[3] Apart from linear excitations (magnons) this equation has nonlinear solutions called kink solitons.[4] Theoretical development and experimental verification of the existence of soliton excitations in quasi-one dimensional systems are rather extensive. In particular, the results of neutron-scattering studies on $CsNiF_3$ (S=1)[5] and $(CD_3)_4NMnCl_3$ (TMMC, S=5/2)[6], nuclear-spin-lattice relaxation and heat capacity measurements on $CsNiF_3$ [7,8], and TMMC [9,10] are interpreted in terms of the SG model.

On the other hand, in a ferromagnetic Ising-Heisenberg quantum chain (S=1/2), the excitation spectrum contains non-linear excitations called bound magnons (BM). These bound magnons resulting from the Ising-like anisotropy were predicted by the pioneer

Hans Bethe.[11] A number of theoretical studies following Bethe's Ansatz reveal that even a small amount of anisotropy may have a drastic influence on the thermodynamics.[12,13] In particular, the work of Johnson and Bonner predicts that under certain experimental conditions thermodynamic properties are almost entirely represented by bound magnons.[13] Despite the theoretical activity, the experimental evidence on these quantum systems is scarce. Besides the earlier experimental study by Haines and Drumheller [14] on CHAC (1-D, S=1/2 Heisenberg ferromagnet), we are aware of only one other experimental investigation done, also on CHAC, $(C_6H_{11}NH_3)CuCl_3$,[15], by Hoogerbeets *et al.*, in which they used ESR to measure energies of the first seven BM levels.

In an Ising system, the elementary excitations are localized spin clusters, where an n-fold spin cluster (bound magnon) is defined as having n adjacent spins which are reversed with respect to other spins. Experimentally, bound magnons in S=1/2, quasi 1-D Ising systems were first observed by Torrance and Tinkam[16] using far-infrared absorption in the effective S=1/2, 1-D Ising ferromagnet $CoCl_2.2H_2O$. Other studies using infrared absorption and ESR to measure the energy levels have since been done in $CoBr_2.2H_2O$ (S=1/2, 1-D ferromagnet)[17] and $RbFeCl_3.2H_2O$[18]. However, to our knowledge no experimental study has been done to investigate the possible effect of bound magnons on the thermodynamic properties of Ising chains. Most of the experimental studies focussed on antiferromagnets and mostly on their static properties, whereas the ferromagnets have received little attention and thus their dynamics are not understood.

The purpose of this thesis is to investigate experimentally the importance of bound magnons in the presently available one-dimensional S=1/2, ferromagnetic systems, FeTAC (Ising like), TMCuC (nearly isotropic Heisenberg), and $CuCl_2$.DMSO (also nearly isotropic Heisenberg). Differential susceptibilities of these compounds have been measured at low temperatures in zero and higher magnetic fields. The data has been analyzed using the Johnson and Bonner theory and also using other expressions such as that of Takahashi and Yamada and of Schlottman in the case of isotropic Heisenberg system at zero field.

Quasi-one-dimensional magnetic materials also have the interesting feature that due to the weak interchain interaction they order at temperatures significantly below the equivalent temperature of the intrachain exchange energy. Consequently, they develop strong short range spin correlations in their "paramagnetic" phase, and exhibit significant spin cluster fluctuations above T_c and below the equivalent exchange energy temperature. In an Ising system spins have discrete symmetry, *i.e.*, a spin either points up or down. Therefore it is possible to stimulate spin cluster flip resonances in this "paramagnetic" phase. Our low temperature EPR results and the observation of spin cluster resonances are discussed in Chapter 4.

One Dimensional Magnetism, Basic Models

A one-dimensional (1-D) magnet is an idealized system in which the spins lie on a chain and interact only with spins on the same chain. However, it is difficult to find such an ideal system for experimental study. In general, linear chain systems that have been synthesized so far do show weak interchain (3D) interaction (quasi one-dimensional). Nevertheless, if the interchain interaction (J') is very small compared to the intrachain interaction (J), (for example, $|\frac{J'}{J}| \sim 10^{-3} - 10^{-4}$) the system can be well-described by a one-dimensional model. In quasi one-dimensional systems, this weak interchain interaction leads to long-range ordering at low temperatures and thus there will be a dimensionality crossover from one to three. However, well above the ordering temperature the long range effect is small and can be neglected and the system can be treated as one-dimensional. Figure 1 illustrates the area of interest.

Next we look at the exchange Hamiltonian which describes the one-dimensional magnetic systems. For a simple case of two interacting spins (dimer) the exchange Hamiltonian is given by:

$$H = -2JS_1 \cdot S_2$$

where J is the exchange constant, which is positive for ferromagnetic exchange and negative for antiferromagnetic exchange.

It is widely accepted that for a system of N interacting spins the isotropic exchange Hamiltonian would have the form:

$$H = -2 \sum_{\substack{i,j \\ i \neq j}} J_{ij} S_i \cdot S_j$$

Considering only the nearest neighbor interaction, a one dimensional anisotropic magnetic system can be represented by

$$H = -2 \sum_{i=1}^{N} \{J_x S_i^x S_{i+1}^x + J_y S_i^y S_{i+1}^y + J_z S_i^z S_{i+1}^z\}$$

The values of J_x, J_y, and J_z define the nature of the exchange coupling. When $J_x = J_y = J_z = J$, the coupling is isotropic in spin space and this case is known as the isotropic Heisenberg model. The extreme situation when $J_x = J_y = 0$ and $J_z \neq 0$ defines the Ising model. Similarly, the case when $J_z = 0$ and $J_x = J_y \neq 0$, leads to an other extreme, referred to as the XY model. The later two cases are anisotropic systems showing easy axis and easy plane anisotropy respectively.

In order to complete the spin Hamiltonian and account for the effect of an applied

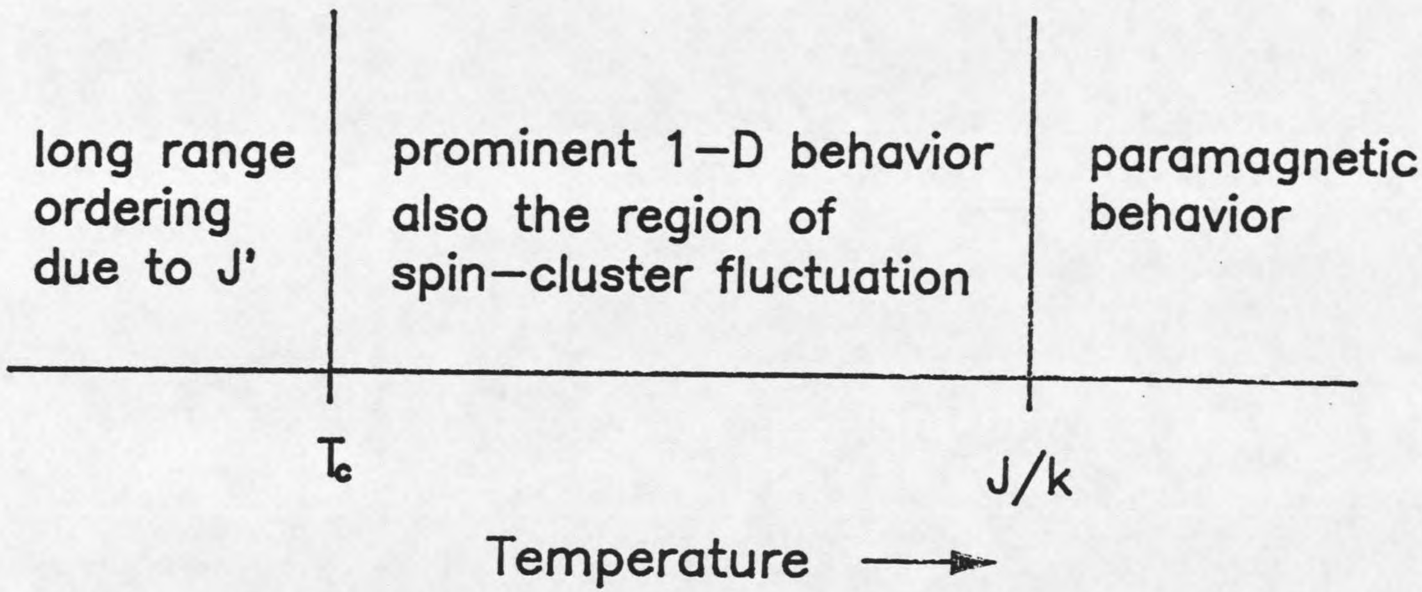

Figure 1. Behavior of a quasi one-dimensional magnetic system.

magnetic field and possible anisotropy (for orthorhombic crystal field) we add the following terms:

Zeeman term: $-g\mu\vec{H}\cdot\vec{S}_i$

Single ion anisotropy term (axial): $D\left[(S^z)^2-\left(\frac{1}{3}\right)S(S+1)\right]$

Single ion anisotropy term (rhombic): $E(S_x^2-S_y^2)$

where the single ion term accounts for the anisotropy arising from the axial crystalline electric field and the rhombic term is from the anisotropy in the plane. D and E are the measure of these anisotropies. For S=1/2 systems (example Cu^{2+}) the single ion term vanishes.

Other Hamiltonians have been used for mathematical convenience but they all give the same results. Among them Johnson and Bonner used the following form:

$$H=-2J\sum_i[S_i^z S_{i+1}^z+\gamma(S_i^x S_{i+1}^x+S_i^y S_{i+1}^y)]$$

where γ is the anisotropy parameter and can vary from γ=1 (isotropic Heisenberg) to γ=0 (Ising).

For experimental purposes, measurements on powders are often sufficient for isotropic or weakly anisotropic materials whereas in the limiting cases (Ising or XY) magnetic measurements along the crystal axes are usually necessary to identify the nature of the anisotropy and to allow comparison with theory.

One-Spin Reversals, Dispersion Relation, Spin Waves

Spin wave theory was first introduced by Bloch in 1930.[19] Let us imagine a Heisenberg ferromagnet in its ground state (T=0). At each lattice site assume there is a localized spin with a spin quantum number S and z-component S^z. In the ground state, all the spins are completely aligned parallel to each other in a preferred direction. Each spin in this state has the maximum allowable value $S^z = S$.

A possible ground state is:

$$|\uparrow\uparrow\uparrow \;.....\; \uparrow\uparrow>.$$

but, infact for the isotropic Heisenberg system the ground state is (N+1) fold degenerate.

As the temperature increases, the system will be excited to a higher energy state. The theory of Bloch showed that at low enough temperatures these excited states can be represented by spin waves (like elastic waves in solids) and as linear combinations of spin waves.. In these excited states a spin wave may be described as a sinusoidal disturbance of the spin system with amplitude at each site proportional to S-S_z. The applications of this to a S=1/2 system will be shown below.

Using Pauli spin matrices an isotropic Heisenberg 1-D system can be described by the Hamiltonian:

$$H' = -\frac{1}{2} J \sum_{ij} \left(\frac{1}{2} \sigma_i^+ \sigma_j^- + \frac{1}{2} \sigma_i^- \sigma_j^+ + \sigma_i^z \sigma_j^z \right)$$

where

$$\sigma_i^{\pm} = \sigma_i^x \pm i \sigma_i^y,$$

$$\sigma_i^z \alpha_i = +\alpha_i, \quad \sigma_i^z \beta_i = -\beta_i$$

where α_i's and β_i's represent the wave functions:

$$\alpha_i = |\uparrow>_i,$$

$$\beta_i = |\downarrow>_i.$$

The ground state is (for N spins):

$$\psi_0 = \alpha_1 \alpha_2 \ldots \alpha_N.$$

This is the state at T=0; it represents the maximum alignment of spins or saturation magnetization. As temperature increases, the system will be excited out of the ground state. The next state may be thought of as one in which a single spin is reversed, however the function

$$\phi_j = \alpha_1\alpha_2 \ldots \alpha_{j-1}\beta_j\alpha_{j+1} \ldots \alpha_N$$

does not diagonalize the Hamilitonian. An eigenfunction ψ_k may be formed by taking a linear combination containing a reversal at a different lattice site:

$$\psi_k = \sum_j C_j^k \cdot \phi_j$$

Substituting this function into the Schrodinger equation $H'\psi_k = E\ \psi_k$ and equating the coefficient of C_j^k we get[20]:

$$\left[E + \frac{1}{2}(N-4)\,J\right]C_j^k + J\ [C_{j+1}^k + C_{j-1}^k] = 0 \tag{1.1}$$

This equation has solutions of the form,

$$C_j^k = N^{-1/2}\, e^{ikja} \tag{1.2}$$

where 'a' is the distance between the spins. This solution represents the wave nature of the excited states (spin waves), i.e., the excited state is equivalent to a spin wave of wave number k. Here the allowed values for k can be determined with the assumption of periodic boundary conditions that require $C_j^k = C_{j+N}^k$: $(Nka)/(2\pi) = 0, \pm1, \pm2, \ldots \pm N/2$. Further substituting (1.2) into (1.1) gives the dispersion relation:

$$E + \frac{1}{2}(N-4)J + 2J\cos ka = 0$$

or $E - E_0 = 2J(1 - \cos ka)$,

where $E_0 = -NJ/2$ is the ground state energy level.

Each of these wave-like quantum states is called a magnon. The magnon energy for small k is given by

$$E_k = \hbar\omega k \approx (\text{const}) \cdot Ja^2k^2$$

As temperature is increased more spin waves are excited. Bloch assumed that the interaction between the spin waves may be neglected and any number of spin waves of a given k can be excited. However this assumption is not accurate.

Actually, spin waves have a repulsive or attractive interaction. For S=1/2, the repulsion results from the fact that there cannot be more than one spin deviation on a given atom. Thus if two spin deviations approach the same lattice site, they will be scattered because of this interaction. The attractive part comes from the fact that the energy of a configuration in which two spin deviations are located on nearest neighbors (bound magnon), is lower than that of a configuration in which the two spin deviations are further apart. In a one dimensional system this can lead to bound spin complexes. This was first pointed out by Bethe.[11]

Two Magnon States and Bound Magnons

As the temperature increases more spins are flipped from the ground state configuration. While the dispersion relation obtained above is true for a single n=1 spin flip, the question arises whether the spin wave picture is valid for $n \geq 2$ (where n labels the number of single spins). Bloch argued that at low temperatures, the presence of a second spin wave cannot seriously modify the derivation of the dispersion law for a second spin wave, and similarly on up to n spin waves, provided n is much smaller than the number N of spins in the sample. Further, Bloch assumed that the eigen function should be very nearly a linear superposition of non interacting spin waves.

Following this picture, the wave function for two spin reversals is:

$$\psi_K = \sum_{l>m} C_{lm}^K \phi_{lm}$$

where, $\phi_{lm} = \alpha_1 \alpha_2 \ldots \beta_l \ldots \beta_m \ldots \alpha_n$

where $K = k + k'$ and K is the total momentum (which is a good quantum number).

Substituting the above into the $H\psi_K = E_K \psi_K$ equation we obtain

$$(E - E^0 - 2g\mu H_0 - 4J)\, C_{lm}^K + J(C_{l,m-1}^K + C_{l,m+1}^K + C_{lH,m}^K + C_{l-1,m}^K)$$

$$= 0 \quad \text{if l, m not neighbors} \tag{1.3}$$

$$= J[C_{ll}^K + C_{mm}^K - C_{lm}^K - C_{ml}^K) \quad \text{if l,m are neighbors}$$

If l,m are not neighbors, a possible solution is

$$C_{lm}^K = e^{iKR} \cos pr$$

with $r = (l+m)a/2; R = (l-m)a$.

This implies that

$$(E - E_0) = E_K(p) = 2g\mu H + 4J(1 - (\cos Ka/2)\cos pa)]$$

with,

$$K = k + k', \quad p = (k - k')/2$$

This can be rewritten as

$$E_K(p) = 2g\mu H_0 + 2J(1 - \cos ka) + 2J(1 - \cos k'a)$$

which represents the sum of the energies of two "non-interacting" spin waves of momentum k and k', where k and k' determined by

$k = \frac{2\pi m + \psi}{Na}, k' = \frac{2\pi m' - \psi}{Na}$ where m and m' are integers < N, and $|m - m'| \geq 2$ and ψ determined by:

$$2\cot\frac{\Psi}{2} = \cot\frac{ka}{2} - \cot\frac{k'a}{2}.$$

If the neighboring spins are reversed, then the non zero term in equation (1.3) would account for bound states. The energy levels for such a bound state can be shown to be:

$$(E - E^0)_{\text{bound}} = 2g\mu H + J(1 - \cos Ka)$$

The derivation of this expression is more complicated and lengthy than for linear spin waves, so we refer the reader to Mattis.[21]

In the limit ka=±π, the magnon and BM energies become:

$$E - E^0 = 2g\mu H + 4J$$

$$(E - E^0)_{\text{bound}} = 2g\mu H + 2J.$$

Note the bound state energy is 2J below the two spin wave continuum and is shown as the solid line in Figure 2. The existence of the lower lying bound magnon states caught the attention of theorists. There has been considerable interest in trying to understand the 2-magnon bound state and possible higher order bound magnons. Exact bound magnon energy levels have been calculated by Bethe[11], Wortis[22] Hanus[23], Majumdar[24], and Reklis and Drumheller[25]. Bethe's solution for an isotropic chain is:

$$E_n(k) = \frac{2J}{n}(1 - \cos ka) + ng\mu H.$$

where n represents the bound spin reversals of n spins. Bethe's work further provides a formalism which involves the bound spin complexes. Although his formalism is complicated and difficult to interpret physically, it serves as a powerful technique to obtain analytical expressions for thermodynamic properties.

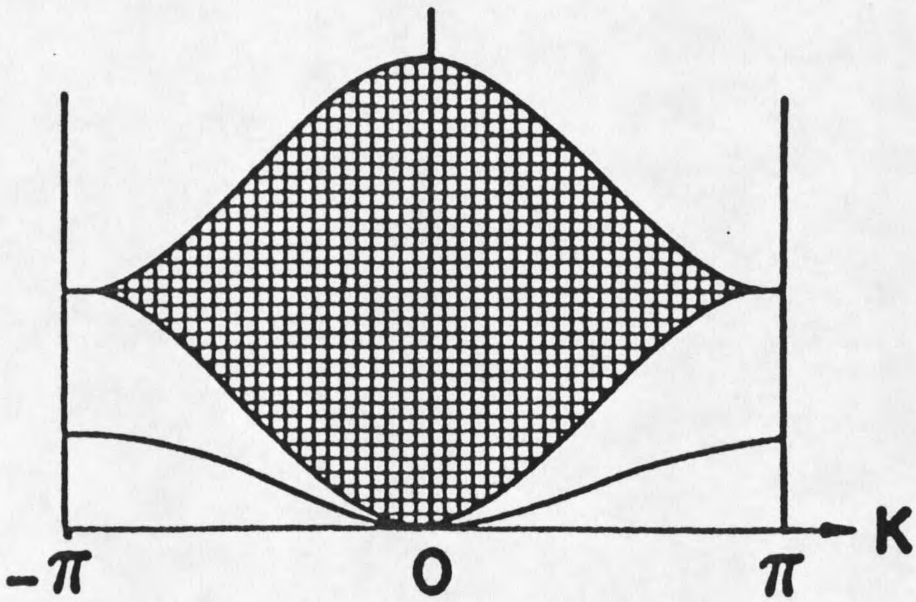

Figure 2. Energy of 2-magnon states in a linear chain. Shading indicates continuum, single line represents bound state.

CHAPTER 2

A SHORT REVIEW OF THE THEORIES

One-dimensional magnetic systems are the simplest systems but still present difficult theoretical problems. Finite chain calculations and high temperature series expansions may be used to understand the thermodynamic properties of these systems at higher temperatures. But the low temperature properties were not clearly understood because of the lack of exact expressions. The difficulty in finding exact solutions gave rise to the application and development of new techniques for solving nonlinear differential equations. Mikeska[3] demonstrated that an easy plane chain of spins ($S > 1/2$) in a magnetic field is equivalent to a sine-Gordon system, which possesses soliton solutions. However, this continuum approximation is not applicable in the quantum limit $S=1/2$. It has been found that Bethe's ansatz formalism is an excellent way to approach this problem, although, due to its complexity, it took several years to develop to a stage where it could be used to derive thermodynamic properties. In particular the work of Gaudin[26] and Takahashi[27] are relevant in this respect. Gaudin was able to express the free energy as an elliptic integral containing an energy function whose form is determined by an infinite set of coupled, nonlinear, integral equations. Extending Gaudin's work, Johnson and Bonner[13] obtained an analytical expression for the low temperature thermodynamic properties of Ising-Heisenberg linear ferromagnetic systems. On the other hand, Takahashi *et al.*, and Schlottmann tried to solve the coupled equations numerically. In this section we review the relevant expressions for the low temperature susceptibility (and specific heat in some cases) of $S=1/2$, isotropic-Heisenberg, Ising-Heisenberg, and Ising linear ferromagnetic systems.

S=1/2, 1-D, Ising-Heisenberg Ferromagnet

Johnson and Bonner Analytical Expression

Johnson and Bonner (JB) used the Hamiltonian:

$$H = -2J \sum_i [S_i^z S_{i+1}^z + \gamma(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y)] - g\mu H \sum_i S_i^z$$

where $0 \leq \gamma < 1$ is the anisotropy parameter, ($\gamma = 0$ for Ising $\gamma = 1$ for Heisenberg). They analytically solved Gaudin's expression for the free energy, which is an infinite set of coupled nonlinear equations, and obtained expressions for the thermodynamic properties at the low temperature limit. For the susceptibility they obtained

$$\chi = T_0^2 \exp\left[-(\Delta^2-1)^{1/2}/T_0\right]\left[4\left\{\frac{H_0^2}{4} + T_0^2 \exp\left(-(\Delta^2-1)^{1/2}/T_0\right)\right\}^{3/2}\right]^{-1} \tag{2.1}$$

$$+ (2\pi T_0)^{-1/2} \exp(-(\Delta + H_0 - 1)/T_0$$

and for the specific heat:

$$C_H = (\Delta^2-1)\exp\left[-(\Delta^2-1)^{1/2}/T_0\right]\left\{\frac{H_0^2}{2} + T_0^2 \exp\left[-(\Delta^2-1)^{1/2}/T_0\right]\right\} \tag{2.2}$$

$$\times\left(4T_0\left\{\frac{H_0^2}{4} + T_0^2 \exp\left(-(\Delta^2-1)^{1/2}/T_0\right)\right\}^{3/2}\right)^{-1}$$

$$+ (2\pi T_0^3)^{-1/2} (\Delta + H_0 - 1)^2 \exp[-(\Delta + H_0 - 1)/T_0]$$

which are valid for $\Delta = 1/\gamma > 1$ and $T_0 << 1$. T_0 and H_0 are defined as $T_0 = (k_\beta T)/2\gamma J$ and $H_0 = (g\mu H)/2\gamma J$. The first term in each of the above expressions is the contribution from the bound magnon (BM) type excitations and the second term is the contribution from the linear spin wave (SW) type excitations. These expressions provide one way to investigate the effect of bound magnons and spin waves on the low temperature thermodynamic properties of 1-D magnetic systems.

The above expressions, obtained from the free energy formalism given by Gaudin, are exact at least at the low temperature limit. The approximation methods involved are complicated and long. However, JB showed that their expressions for the susceptibility and specific heat can be obtained from a simplified physical argument.[28] In JB notation, the zero-temperature dispersion curves for the S=1/2, 1-D, Ising-Heisenberg ferromagnet are given by

$$E_n(P) = nH_o + \sinh\phi(\cosh n\phi - \cos P)/\sinh n\phi$$

where $\cosh\phi = \Delta = 1/\gamma$, n=1,2,...... and P is just a number that satisfies $0 \leq P \leq 2\pi$. The P's are distributed uniformly between 0 and 2π and for a given n, obey a Fermi-like exclusion principle. The n=1 excitations and a linear combination of the n=1 excitations are spin waves and higher-n excitations are bound states of spin waves. The energies of the first excited states are $E_1(q) = H_o + \Delta - \cos q$. There are N such states with $q = 2\pi m/N, 0 \leq m < N$. When these states and their degeneracies are used to form a partition function, and the thermodynamic functions are calculated, it gives an expression which is exactly the same as the spin wave term in the above expressions. Accordingly the thermodynamic functions obtained from using the high n-bound states, after making low-temperature approximation, give the bound magnon term in the above expression.

Since we are interested in the susceptibility measurements and the comparison with JB theory, the expression for χ is plotted in Figures 3(a)-3(c) to demonstrate the behavior of the susceptibility as a function of field, temperature and the anisotropy parameter γ. Recall the expressions given by Johnson and Bonner are unitless. Looking at these expressions at the high temperature limit at zero field and comparing with the Curie-law one can find the unit conversion factor to be $N_A g^2\mu^2/2\gamma J$. All these theoretical curves shown are the JB susceptibility expression multiplied by this conversion factor.

Figure 3(a) shows $\chi vs T$ in fields of 0, 1, 1.5, and 2 Tesla. The solid lines are drawn for the parameter J/k = 45K, g=2.1, and $\gamma = 0.95(5\% anisotropy)$ and represent the total contribution of both SW and BM. The behavior of χ is distinctive, showing a broad maximum at higher field. Also the maxima at higher fields occur at relatively higher temperatures. These maxima are not related to any ordering phenomena, but rather are due to the freezing out of dynamic modes. Figure 3(b) shows the temperature dependence of the SW, BM, and total contribution separately at H=1 Tesla. It is clear that the maxima are almost entirely due to the BM contribution to the susceptibility. The SW term gives very little contribution and can be almost neglected. Figure 3(c) shows $\chi vs T$ for different anisotropy parameters γ. Note that the location of the maxima is sensitive to γ. A further description of the JB expressions and a summary of calculations based on these expressions can be found in Donald N. Haines's Ph.D. thesis (1987).

In the Ising limit the Johnson and Bonner expression for the susceptibility exactly follow the Ising expression given by Fisher (see the section below). However, the Johnson and Bonner theory is not valid at the exact isotropic Heisenberg limit. The only available expressions for S=1/2, isotropic Heisenberg systems are of Takahashi and Yamada[29], and of Schlottmann[30]. They approached this limit numerically and used the Hamiltonian:

$$H = -J \sum_i \left[S_i^z S_{i+1}^z + S_i^x S_{i+1}^x + S_i^y S_{i+1}^y - \frac{1}{4} \right] - 2H \sum_i S_i^z$$

Compared to the JB Hamiltonian, there is a factor of 2 in the Zeeman term and J is used for the coupling constant instead of the usual 2J. Therefore, care must be used when comparing this expression with other expressions for the susceptibility. It turns out that we need to multiply the expression for the susceptibility by a conversion factor $N_A g^2 \mu^2/4$.

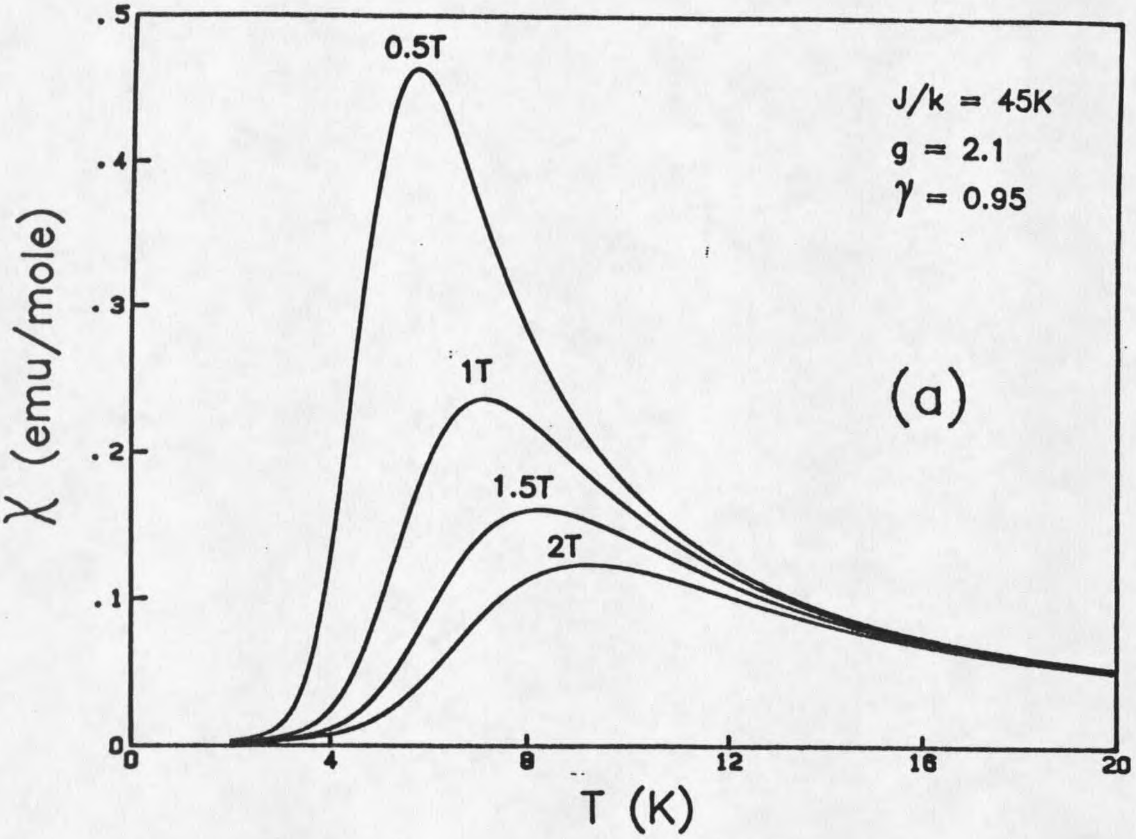

Figure 3. Johnson and Bonner susceptibility as a function of temperature for J/k=45K, g=2.1:

(a). at different magnetic fields for $\gamma = 0.95$. The solid lines represent the total (SW+BM) contribution to the susceptibility.

(b). at 1 Tesla for $\gamma = 0.95$. The contributions from spin waves (SW), bound magnons (BM), and total (SW+BM) are drawn separately.

(c). for different values of γ at 1 Tesla.