Heisenberg Antiferromagnet

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Abstract

The Heisenberg model is described. Some of the interesting behavior of Heisenberg antiferromagnets and its behavior as a function of dimension is described. One dimensional systems have no long range order, two dimensional systems order magnetically only at zero temperature, and three dimensional systems have a non-zero critical temperature. Assembling lower dimensional pieces into ladders and multilayers is especially interesting, since the behavior of the system depends on whether it is composed of an even or an odd number of pieces. An early numerical method of solution, the high temperature expansion is also explained.

1 Introduction

A magnetic system can be modeled as a lattice of spins which interact with the applied magnetic field, and with each other. Spins interacting with a magnetic field H have the Hamiltonian[1]

$$Ha = -g\mu_B \sum_{i=1}^{n} \mathbf{S}_i \cdot H. \tag{1}$$

The simplest model of a ferromagnetic system is the Ising model. In the Ising model, spins can either point parallel or antiparallel to the magnetic field. The nearest neighbor spins interact with each other through the Hamiltonian

$$Ha = -J \sum_{\langle i\ j \rangle} S_{ix} S_{jx}, \tag{2}$$

where $\langle i\ j \rangle$ indicates that the sum is only over adjacent spins. S_x is either +1 or -1. The Ising model is named after Ising who solved it exactly for a one dimensional lattice in 1925. Onsager solved the two dimensional Ising model exactly for zero applied magnetic field in 1944. The Heisenberg model is similar except that the spins are three dimensional; they can point in more than just two directions. In the classical Heisenberg model, the S components can take on any value between -1 and +1. The spin interaction component of the Hamiltonian is

$$Ha = -J \sum_{\langle i\ j \rangle} (S_{ix} S_{jx} + S_{iy} S_{jy} + S_{iz} S_{jz}). \tag{3}$$

This model can only be solved exactly on a one dimensional lattice with zero applied magnetic field. This classical model is a good approximation to the quantum mechanical Heisenberg model near T_C. The classical model is equivalent to the quantum mechanical model with infinite S. At low temperature, this model is very different from the finite S result. The quantum mechanical Hamiltonian for a Heisenberg antiferromagnet is

$$Ha = J \sum_{\langle i\ j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \tag{4}$$

where **S** is a three component spin operator with 2S + 1 discrete orientations. An exact solution by Bethe in 1931 showed that there is no long range antiferromagnetic order for a one dimensional chain[2]. However, long range order is predicted for a $S = 1/2$ antiferromagnetic material with a square lattice.

Another related model that is of interest is the spherical model. This model is equivalent to letting the spins have an infinite number of components, rather than the three components of the Heisenberg model or the single component of the Ising model. This spherical model is unphysical, but can be solved in one, two, or three dimensions with and applied magnetic field. In addition, critical-point exponents can be found exactly in higher dimensions[1].

The quantum mechanical Heisenberg model presents a more difficult problem, but can be used to model real magnetic materials provided that the materials have well localized spins and the interactions are isotropic. EuO and EuS meet these conditions. This model provides a good description of the antiferromagnetic material $RbMnF_3$[1]. The most interesting materials that are well described by the Heisenberg model are closely related to high temperature superconductors. The cuprate insulators which can be doped to produce superconductors are excellent examples of two dimensional spin one-half antiferromagnets that can be described by the Heisenberg model. The multilayer Heisenberg antiferromagnet model can aid in the understanding of the magnetic properties of high temperature cuprate superconductors which contain several weakly coupled copper oxide layers.

The quantum mechanical Heisenberg model is especially interesting because low dimensional systems exhibit a wide range of surprising physical behavior. Coupled one dimensional chains behave very differently depending on whether the number of coupled chains is odd or even. Coupled planes also show different behavior depending on whether there is an odd or an even number of multilayers. When even numbers of coupled chains are doped, they exhibit hole pairing. This pairing is similar to a "d-wave" state, which leads to very different behavior from the Luttinger liquid behavior of odd numbers of doped, coupled chains. In Luttinger liquids the spin and the charge part of the added holes are separate, and move at different velocities. Doped materials composed of an even number of coupled chains might exhibit superconductivity[3].

2 Numerical Methods

The high temperature expansion is one of the simplest numerical methods used to study the Heisenberg antiferromagnet. In this method, the partition function is expanded as a power series

$$Z_N(T,H) = Tr\{e^{-\beta H_a}\} = Tr(1)\{1 - \beta tr(H) + \frac{1}{2}\beta^2 tr(H^2) + \ldots\}[1] \tag{5}$$

$$\text{where } tr\ H^l \equiv \frac{Tr\ H^l}{Tr(1)}, \text{and } Tr(1) = (2S+1)^N \tag{6}$$

Using these equations, the Gibbs free energy can be calculated

$$G(T,H) = -k_B T \ln Z_N(T,H) \tag{7}$$

$$= -k_B T[\ln\{Tr(1)\} + \ln\{1 - \beta tr(H) + \frac{1}{2}\beta^2 tr(H^2) + \ldots\}] \tag{8}$$

$$= -k_B T \sum_{l=0}^{\infty} \left(\frac{c_l}{l!}\right) \beta^l \tag{9}$$

The coefficients c_l are called cumulants. The high temperature expansion is essentially an expansion in J/k_BT, with each cumulant contributing to order J^l. The physical significance of this is that the l th cumulant considers all possible paths involving l interactions by which a spin can interact with its nearest neighbor. The first few cumulants can be calculated easily, but additional terms become increasingly difficult to calculate. The high temperature expansion is much simpler for the classical model than the quantum mechanical model. Critical exponents appear to be independent of S, but the critical temperature is not. In 1958, Rushbrooke and Wood correctly calculated the first seven terms in the high temperature expansion for quantum-mechanical Heisenberg model with arbitrary spin S. These terms are not just used directly; extrapolation methods are used to estimate the behavior of the infinite series. Simply truncating the expansion, will produce a polynomial. Since polynomials do not diverge, critical behavior can not be examined without extrapolating. The radius of convergence of the power series is the important quantity (assuming the closest singularity to the origin is the physical singularity). If the terms decrease as 1/l the ratio test for convergence can be used to estimate the radius of convergence. When nonphysical singularities are encountered, the method of Padé approximants is often used. Sometimes nonphysical singularities can be removed by expanding about a different variable (e. g. $\tanh(J/k_BT)$ instead of J/k_BT).

Determining Padé approximants consists of fitting the function to a ratio of two polynomials rather than a single polynomial. The order of each of the two polynomials can be varied, as long as the sum of the two orders is less than or equal to the order of the known terms in the series to be approximated. Usually each Padé approximant contains one pole near the critical point and the residue at that pole predicts the critical exponent. The average of these approximate values is used as an estimate for the true value.

3 Increasing Dimensions

The most interesting thing about Heisenberg antiferromagnets is that putting together an odd number chains to form a two dimensional "ladders" gives different results than if an even number of chains are put together. A similar effect happens when planes are put together as multilayers to make a three dimensional model. A single chain with half-integer spin does not have long range antiferromagnetic order, instead the spin correlations decay inversely with the distance between the spins. Ladders composed of an odd number of chains (with half-integer spins) behave similarly to single chains. Spin correlations decay as a power law with logarithmic corrections. The ground state (doublet) of these ladders is the same as that of a single chain with a different effective coupling constant J.

The ground state of a rung of a ladder composed of an even number of chains is the singlet state. However, the spin correlations are only short-ranged. These correlations decay exponentially because there is a spin gap. There is a finite energy separating the S = 0 ground state, and the first excitation (S = 1) in the infinite ladder. This is significantly different from the gapless ladders composed of an odd number of chains. For ladders composed of two chains this spin gap is about 0.5J, for four leg ladders, results have been obtained which range from 0.12J to 0.27J. This behavior is similar to the behavior of a single chain composed of integer spins. Chains with integer spin have finite correlations lengths, and a spin gap.[3]

Ladders with odd and even numbers of chains can be investigated experimentally as well. $(VO)_2P_2O_7$ forms two leg ladders, which have been measured experimentally. The coupling constant along the chains was measured to be 7.76 meV and the coupling along the rungs was 7.8 meV [4](These values are obtained by fitting the susceptibility vs. temperature). Spin gap of these ladders was measured by inelastic neutron scattering to be 3.7 $\pm$ 0.2 meV; this is very close to the theoretical value of 3.9 meV.[3] One of the most useful compounds to study is $Sr_{n-1}Cu_{n+1}O_{2n}$. The number of chains which form a ladder of this material depends on the value of n. $SrCu_2O_3$ forms a ladder of two chains, and $SrCu_3O_5$ forms a ladder composed of three chains. At low temperature, the susceptibility can be described as $\chi(T) \sim \frac{e^{(-\Delta_{spin}/T)}}{\sqrt{T}}$, where Δ_{spin} The coupling constants for $SrCu_2O_3$ are close to isotropic with values close to 1300 K. The spin gap should be about 650 K, but fits to the low temperature susceptibility yield a spin gap of 420 K[5]. However, Nuclear Magnetic Resonance measurements indicate an activation energy of 680 K[3]. C-axis coupling between layers of ladders might be explain this difference. C-axis coupling can also account for the discovery of long range antiferromagnetic ordering below 52 K in three chain ladders of $SrCu_3O_5$. Long range magnetic order has not been found in ladders composed of only two chains. The magnitude of the spin gap decreases as the (even) number of chains increases. This behavior is expected, since in the large n limit, it should not matter whether n is even or odd. The two dimensional square lattice Heisenberg model (regardless of the value of the spins) has a ground state with long range antiferromagnetic order, and no spin gap. This order is destroyed by thermal fluctuations for temperatures above absolute zero.

Assembling two dimensional layers into multilayer systems produces results which are similar to the two dimensional ladders. Again, the results are very different depending on whether there is an even or odd number of layers in the system. The spin-S bilayer has been studied extensively, and found to have a second order transition between a Néel phase and a dimer phase. Multilayer spin 1/2 systems are a topic of current research. A multilayer system can be described by the Hamiltonian:

$$Ha = J_1 Ha_{plane} + J_2 Ha_{rung}, \tag{10}$$

$$\text{where } Ha_{plane} = \sum_{\alpha=1}^{n} \sum_{<i,\ j>} \mathbf{S}_{\alpha,\ i} \cdot \mathbf{S}_{\alpha,\ j}, \tag{11}$$

$$\text{and } Ha_{rung} = \sum_{i} \sum_{\alpha=1}^{n-1} \mathbf{S}_{\alpha,\ i} \cdot \mathbf{S}_{\alpha+1,\ i}[6] \tag{12}$$

Layers are indexed by alpha, and sites by the indices i, and j. For $J_2 << J_1$, the model describes n weakly interacting planes. For $J_2 >> J_1$, the model describes weakly coupled "rungs" of a three dimensional ladder, with each rung consisting of n spins.

Systems with an odd number of layers can be mapped to the single layer antiferromagnet if J_2 is large. A similar system with an even number of layers has a gap if $J_2 >> J_1$. If $J_2 << J_1$, the odd layered system can be mapped to the Ising model with the additional spin components considered as a perturbation. If $J_2 >> J_1$, the eigenstates of the rung (with a doublet ground state) can be taken as basis states for an Ising expansion. The resulting series can be extrapolated to the isotropic limit, by doing a variable transformation and then using Padé approximants. These estimates predict long range antiferromagnetic order and no spin gap for all values of J_1/J_2[6].

Systems with an even number of layers can be investigated by means of an expansion in J_2. For large J_2, the system behaves as a disordered spin liquid. At some critical ratio of J_1/J_2, the system undergoes a second order transition, resulting in an ordered magnetic state with no spin gap. H_{rung} can be taken to be the Hamiltonian with Hplane treated as a perturbation. Again, Padé approximants can be determined for the resulting series. This method results in a critical value of J_1/J_2 which scales with the number of layers as $0.913/n - 0.250/n2$ [6].

Recent Monte Carlo simulations of the three dimensional spin 1/2 Heisenberg antiferromagnet on a simple cubic lattice indicate a critical temperature $T_c/J = 0.946 \pm 0.001$[7]. This value agrees with analytic calculations. These results are consistent with the classical Heisenberg universality class. This ordering at finite temperature confirms the predictions of stronger long range order in three dimensional systems than in two dimensional layers.

4 Conclusions

The behavior of Heisenberg antiferromagnets is very interesting, in that these models exhibit a wide range of physical behavior. Current methods of investigation are much more sophisticated and accurate than the high temperature expansion. However, the basic idea behind other expansions in the same. Approximations and simulations of the Heisenberg model are particularly valuable, because the model cannot be solved exactly except in the simplest of cases. These theoretical investigations agree with experiment, and many unique phenomenon can be observed experimentally.

References

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