Upper Bounds on the Magnetization of Ferromagnetic Ising Models

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Abstract

Upper bounds on the magnetization of arbitrary ferromagnetic spin models are investigated. We discuss two methods by which it was proven that the mean field magnetization was shown to be an upper bound on the true magnetization. These are the Pearce and Slawny proofs. Results are given on analyses of methods attempting to extend the Pearce proof.

Extensions to mean field theory are studied. We present new results which show that two of these extension methods also give upper bounds on the magnetization. We prove that the two-body extension, the Oguchi method, is an upper bound for spin $1/2$ Ising models. For those spin $1/2$ models where the three-body method predicts a unique magnetization, this too is proven to give an upper bound. The corresponding critical temperatures are proven to fall in the decreasing sequence

$$T_c(mean\ field) \geq T_c(Oguchi) \geq T_c(3\text{-}body) \geq T_c(true)$$

where the inequalities are strict if the extension schemes are effectively used. As applications of these methods, we obtain graphical spontaneous magnetization curves for various models and the new upper bound $T_c \leq 2.897$ for the one dimensional $1/r^2$ Ising model, improving the previous mean field upper bound of $T_c \leq 3.290$.

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Chapter 1

Introduction

I.1 The Physical Question

Consider the following physical experiment. Place a piece of iron with zero magnetization, $m = 0$, in a heat bath at temperature T. Apply an external magnetic field h, $h \geq 0$, to the iron and slowly decrease this field until $h = 0$. Measurement of the magnetization would now give $m = 0$ if T was sufficiently large and $m > 0$ if T was sufficiently small. This is the ferromagnetic example of a first order phase transition with m serving as the order parameter. The magnetization at zero external field is called the spontaneous magnetization. The temperature above which the spontaneous magnetization is zero and below which the spontaneous magnetization is non-zero is called the critical temperature T_c. Figure 1 shows an experimental spontaneous magnetization curve.

From a physics point of view, one very interesting feature in the above experiment is the kink or non-smoothness in the m vs. T graph. With most of our microscopic physics showing smooth behavior, we are led to wonder if our understanding of statistical mechanics and fundamental interactions are sufficient to create a model that manifests such non-smooth behavior. We create such a model by abstracting only the (apparently) most important properties of the physical system. The dominant cause of ferromagnetism is the apparent alignment of atomic dipoles and the tendency of dipoles to align themselves with an external field. We know these atoms lie in a lattice and believe ferromagnetism to be basically independent of the size or shape of the lattice. These considerations led to the creation of the Ising model in 1920 by Wilhelm Lenz. The model was first analyzed by Lenz's student Ernst Ising in the same year.

In the Ising model our basic object is a spin variable s_i which takes values in the space $\Omega = \{ -1,1 \}$. The subscript 'i' denotes which site in the lattice Λ the spin variable s_i is attached to.

We introduce interactions by means of a Hamiltonian $\mathbf{H}$,

$$\mathbf{H} = -\sum_{i,j\,\varepsilon\Lambda} J_{ij} s_i s_j - h \sum_{i\varepsilon\Lambda} s_i \tag{I.1}$$

and cause alignment to be a favorable configuration by demanding the pair coupling J_{ij} , and the external magnetic field h, to be non-negative. We then say we are working with a ferromagnetic system. For most applications it is assumed the coupling is translation invariant, i.e.,

$$J_{ij} = J(|i-j|)$$

We also assume the total coupling of any one spin to the outside world is finite, i.e., $\sum_j J_{ij} < \infty$, in order to get interesting behavior. Our convention is that the self-coupling of any spin, J_{ii}, is zero. Our lattice Λ is usually some finite subset of $\mathbb{Z}^d$ although other structures, e.g., triangular or hexagonal lattices, are allowed. The statistical mechanics of a finite lattice Λ is introduced by defining expectations using the Boltzmann factor:

$$\langle f \rangle_{\Lambda,\mathbf{H}} = \left[\sum_{[s]} f\, e^{-\beta\mathbf{H}}\right] / \mathbf{Z}$$

where

$$\mathbf{Z} = \sum_{[s]} e^{-\beta\mathbf{H}}$$

is the partition function. Here β is the inverse temperature $1/kT$. $\sum_{[s]}$ stands for a configuration sum where the spins $s_i \,\varepsilon\, \Lambda$ assume all their possible values. The measure assigned to any spin configuration is $\bigotimes_{i\varepsilon\Lambda} d\mu_i(s_i)$; for this model $d\mu_i(s) = \frac{1}{2}\{\delta(s-1) + \delta(s+1)\}$ is the normalized counting measure. For translation invariant couplings in a finite lattice boundary conditions must be prescribed. Typical ones are plus-boundary conditions, where spins in $\mathbb{Z}^d \setminus \Lambda$ are fixed to be plus $(s_i = +1)$ (see figure 2.a); periodic boundary conditions, where couplings of spins to spins in $\mathbb{Z}^d \setminus \Lambda$ are understood to apply to spins 'on the other side' of Λ (see figure 2.b); and free boundary conditions, where couplings to any spins in $\mathbb{Z}^d \setminus \Lambda$ are set equal to zero (see figure 2.c). It is mathematically convenient to get rid of any dependence on the size or shape of Λ by taking the thermodynamic limit of expectations. This means we allow the size of Λ to go to infinity, $|\Lambda| \to \infty$, and define the true expectation value as

$$\langle f \rangle_{\beta,\mathrm{H}} = \lim_{|\Lambda| \to \infty} \langle f \rangle_{\beta,\mathrm{H},\Lambda}$$

Often specific parameters of H, such as the magnetic field h, will be written as subscripts instead of H when we wish to emphasize their presence. Subscripts may also be omitted when their presence is clear from context. We arrange for $|\Lambda| \to \infty$ by taking a growing, nested sequence of cubes whose length approaches infinity. Our original problem is now an investigation of

$$m(\beta) \equiv \lim_{h \to 0^+} \langle s_i \rangle_{\beta,\mathrm{H},0}$$

or

$$m(\beta) \equiv \lim_{|\Lambda| \to \infty} \langle s_i \rangle_{\beta,\Lambda,+}$$

where the 0 subscript denotes free boundary conditions, and the $+$ subscript denotes plus boundary conditions. By general arguments, these two definitions are equivalent [1]. Since the equilibrium state of our system in the thermodynamic limit is usually translation invariant, the 'i' dependence in the expectation is usually non-existent. Attention must be paid, though, to the 'i' dependence in the intermediate calculations when Λ is finite.

The demonstration that the Ising model exhibited the ferromagnetic phase transition came in two steps. First, in 1936 Rudolf Peierls gave an argument which showed that the spontaneous magnetization was non-zero at sufficiently low temperature [2]. He used plus boundary conditions on a two dimensional square lattice with nearest neighbor couplings, i.e., $J_{ij}=0$ if j is not a (geometric) nearest neighbor to i. In the Peierls argument one relates the probability of a minus spin $(s_i = -1)$ to the probability of a contour on the lattice. By comparing the energy cost of having a contour to the gain in entropy from a contour, Peierls is able to find a temperature below which the probability of a minus spin is less than $1/2$, and therefore that the spontaneous magnetization is positive. The second part of the demonstration came in 1967 from Robert Griffiths who showed that for lattices of any dimensionality the spontaneous magnetization was zero at a sufficiently high temperature [3]. He used a 'ghost spin' trick and compared the magnetization to various correlation functions to find that for sufficiently high temperature, the magnetization is less than some linear function of the external field. This implies that the spontaneous magnetization must be zero. To round out these two arguments into a magnetization graph, we use a correlation inequality called GKS II which tells us that correlation functions don't decrease as the temperature is lowered and don't increase as the temperature is raised. GKS II also tells us that if you have a non-zero magnetization in dimension d, you also have non-zero magnetization in dimension $d+1$. We then know that a three dimensional Ising model has the appropriate ferromagnetic behavior and can be used as a model for real ferromagnets. Were the two temperature bounds from the Peierls argument and the Griffiths argument the same, we would know the exact transition temperature. Since these two temperatures are not the same, we have two bounds on T_c, a lower bound and an upper bound. A theoretical magnetization curve is shown in figure 3 and we indicate what we have learned by these analyses on this figure.

While we have shown the Ising model to have the simplest property of figure 1, that of regions of positivity and of zero-ness, we may inquire about some other features of figure 1. The apparent continuity of the graph is partially shown by GKS II. GKS II allows one to show monotonicity of m as a function of T, and thus continuity almost everywhere. As one might believe this to be insufficient, we point out that the one dimensional $1/r^2$ (where $J_{ij} = |i-j|^{-2}$) Ising model is believed to possess a discontinuity right at the transition temperature. The concavity of $m(T)$ above T_c is easy to show (the graph is flat); the concavity below T_c or piecewise concavity of $m(T)$ everywhere is as yet an open question. The problem of determining m as a function of T is very much open and is of major importance in using the Ising model as a quantitative explanation for any physical phenomenon. The next several chapters describe work and partial results towards answering this question.

Attention has so far been focused on the ferromagnetic phase transition. We wish to point out that there are other kinds of phase transitions and reasons to study the Ising model. Most common is the liquid - gas phase transition of water. The order parameter is the density of the mixture of water and water vapor. The critical temperature of water is $374°C$ at a critical pressure of 217.72 atmospheres. Other examples include the superconducting / normal states of some metals and the superfluid states of helium. The most recent source of interest has been the conjectured quark deconfining transition of the vacuum. It is believed that the universe is in a low temperature phase where quarks are permanently confined, but that there exists a high temperature phase where quarks are free. This question originated in quantum field theory but similarities in the mathematical treatments have re-awakened interest in the study of Ising-like models in statistical mechanics, specifically lattice gauge theories. A different reason to study spin systems is the universality hypothesis for critical exponents. By solving for the critical exponents of more types of spin models, one will better understand the range of validity and necessary conditions for universality.

Our last word in this chapter is a warning. While the physical ideas behind the Ising model underlie many physical systems, it takes further work to relate the Ising model properties to the real world properties. Appropriate dimensional quantities must be inserted and the hypotheses behind the Ising model must be checked for validity. For example, does the spin-spin interaction really dominate the Hamiltonian so much that other interactions may be neglected? With this caveat in mind, we focus attention on a study of the Ising model itself.

I.2 First Analyses: Solutions and Approximations

Many variations on the original Ising model have since been introduced. Their utility lies both in a possible closer modelling of some real world systems and their amenity to some kinds of mathematical analysis. Insofar as we can learn something from them they increase our understanding of the mechanics and general properties of phase transitions. Already mentioned is the possibility of changing the underlying lattice structure. Real crystals can have one of 32 point groups associated with them and we desire at least this much freedom in specifying our models. It turns out that the qualitative features of phase transitions depend mainly on the dimensionality of the lattice and not on the particular lattice used; quantitative features will depend on the type of lattice used. Our spin space $\Omega = \{ -1, 1 \}$ corresponds to a spin $1/2$ or two state system. Higher angular momentum spins, the spin $n/2$ models, have spin spaces

$$\Omega = \{ -1 , -1+\frac{2}{n} , -1+\frac{4}{n} , \cdots , 1 \} .$$

The spin - spin interaction is still taken to be $-J_{ij}s_is_j$. The plane rotor (also called the x - y or O(2)) model imagines each spin to be a two component vector having components (x,y) satisfying $x^2+y^2=1$ with the spin - spin interaction being $-J_{ij}\vec{s}_i \bullet \vec{s}_j$. This introduces the n-vector models where each spin is a normalized n-component vector with the dot product interaction. The Heisenberg model is the three vector model and is much studied since it is a three dimensional spin. Clock (also called $\mathbf{Z}_p$) models are discretized versions of the x - y models. Instead of letting the components (x,y) run over the continuum of their allowed values, only certain ordered pairs are allowed, e.g. the $\mathbf{Z}_4$ model allows the spin to point to the number 12, 3, 6, and 9 on a clock. The interaction in all the above models need not be pair couplings. Terms like the three body coupling, $-J_{ijk}s_is_js_k$, or many body couplings may be put into the Hamiltonian. Theories with four body terms are in use in the study of lattice gauge theories [4]; there the interaction is $-J \prod_{i \epsilon plaquette} s_i$. The most important feature of pair couplings appears to be the rate of decay of the coupling at long distances. For example, nearest neighbor couplings in a one dimensional spin $1/2$ model cause no transition, but $J_{ij} = |i-j|^{-1.5}$ do. This is why people distinguish between finite range couplings, where if the distance between sites i and j is too large, $J_{ij}=0$, and long range couplings, where if one goes out far enough away from site i one can always find a non-zero J_{ij}. Apart from the above models, there is still a plethora of models that we shall not discuss, e.g., Potts, Villain approximation models, solid on solid, spherical, etc. It should also be mentioned that there are antiferromagnetic models, J_{ij} and h may assume negative values. These are of interest nowadays in the discussion of spin glasses and the RKKY interaction [5]

$$J_{ij} \sim \frac{\cos|i-j|}{|i-j|^3}.$$

The proofs of many results useful in analyzing general ferromagnetic spin models fail when antiferromagnetic couplings are allowed, and we defer study of antiferromagnetic models to a later date. The above models are also classical in the sense that we do not worry about commutativity of any of the spin variables. Quantum analogs of all the above models exist but we shall not discuss them here.

The first analysis of the Ising model was done in 1925 by Ernst Ising (appropriately enough) for his graduate studies. His conclusion that the one dimensional nearest neighbor spin $1/2$ Ising model had no phase transition was rather disappointing. It had been hoped that this model would explain ferromagnetism and that was one of the reasons for its creation. However the method nowadays used to solve one dimensional problems is quite interesting and proves versatile enough to handle discrete spin spaces with finite range coupling. All these models possess no phase transition. The method is called the transfer matrix method and basically enumerates all the possible states of a spin and its effective neighbors, then uses matrix multiplication to extend the configuration sum to any finite size chunk of a one dimensional lattice. The partition function for finite Λ is found to depend on the eigenvalues of the transfer matrix. In the thermodynamic limit only the largest eigenvalue is important and it becomes easy to show that the thermodynamic functions are smooth and there is no phase transition. The same method together with lots of mathematical manipulations was used by L. Onsager in 1944 to calculate the partition function for the two dimensional spin $1/2$ nearest neighbor zero external field Ising model [6]. In the famous Onsager solution, he shows directly that there is a phase transition in two dimensions and finds the critical temperature to be $T_c = 2.269$ (in units where the coupling constant equals 1). Variations of the Onsager solution have been made to solve other two dimensional lattices exactly;

examples include the triangular and hexagonal lattices. Extensions of the transfer matrix analysis have been attempted for higher dimensional lattices but these have so far been unsuccessful in solving these models. A distinct two dimensional model, called the ice model, was solved by Elliot Lieb [7], also by using the transfer matrix method. An enhanced version of the ice model, called the 8 - vertex model, was solved by R. J. Baxter [46]. This rounds out the list of types of major exactly solved models.

Since we are only able to solve a few models, and many of those solutions are quite complex, it is natural to seek approximate methods of analysis which are simpler, and which work in greater generality. We list a partial set of such methods. Examination of the form of expectations leads one to a high temperature (small β) expansion [8]. This is done by expanding the Boltzmann factor into its Taylor series. For nearest neighbor models this becomes a sum over self avoiding walks on Λ (see [9]). Duality is a method which relates one Hamiltonian on a lattice to a possibly different Hamiltonian on a (possibly) different lattice [10]. When duality relates a theory to itself, it also allows a high temperature expansion to be related to a low temperature expansion. One then gets a guess at the value of T_c by saying it is at the (assumed) common singularity of these two expansions. Since the two dimensional theories solved to date have had only one critical point, duality has succeeded in correctly predicting the value of T_c. Monte Carlo techniques have been used to calculate spin correlation functions [11]. The method hopes to be able to choose a small representative sample of spin configurations and compute on the basis of these, rather than having to deal with the large number of all possible spin configurations. This method is ideally suited to the large computing capability being offered by modern computers, and with correct Monte Carlo programs, offers the possibility of better answers with more computing time. Renormalization group analyses have been tried. The rigorous applications include analyses of Dyson's hierarchical model [12] and the Kosterlitz - Thouless transition in two dimensional x-y models [13]. One believes lack of a fundamental length scale to be characteristic of all systems near their transition point and this idea is precisely what the renormalization group tries to capture. The Curie-Weiss molecular field theory, also called mean field theory, was an approximation that tried to make self consistent solutions to spin models (see chapter II). The great virtue of this method was that it predicted phase transitions and gave a reasonably easy equation to solve to get the transition temperature. Unfortunately this theory turns out to have a habit of predicting too many phase transitions and will sometimes predict a phase transition where there really isn't one. We can understand this intuitively by looking at phase transitions as a macroscopic manifestation of microscopic cooperative effects. In the unmagnetized phase each spin prefers to point in any direction independently of the other spins, resulting in an overall spin expectation value of zero. In the transition to the magnetized phase, spins will see other spins preferentially pointing in some direction and will want to point in that direction too. This process cascades through the lattice and one gets a non-zero magnetization. Important in this argument is the ease by which a spin cooperates with all the other spins. This information is contained in the spin-spin correlation function. The real spin system has to contend with intervening spins sometimes not pointing in the same direction as spins further away. These are called fluctuations and cause information to be inefficiently propagated through the lattice, thus making cooperation and phase transitions hard. Mean field theory on the other hand has perfect correlation between all of its spins. This makes cooperation much easier, thus explaining the ease of having a phase transition in this model. This also explains why the mean field magnetization should be greater than the true magnetization. We shall prove this to be true in

Chapters IV and V. Mean field theory is the first in a series of approximations collectively known as the Cluster Variational approximations. We shall discuss these at greater length in chapter II.

A wealth of data has been amassed using these techniques on many different models [14]. We are led to wonder, though, are these numbers, e.g., the approximations to T_c, above or below their true value and how good are they as best guesses to the true value? On the one hand most of the figures obtained in this manner have agreed well with exact results when we have both figures. On the other hand we are without a guide as to what to do if there happen to be two conflicting best guesses. A case in point is the presently studied random field Ising model. Researchers are trying to determine the lower critical dimensionality, d_c, of the model, i.e., the lowest dimension in which there is a phase transition. There are conflicting arguments saying that $d_c = 2$ (see reference [15]) and $d_c = 3$ (see reference [16]). If all arguments are both reasonable and sound, the deciding factor must be a rigorous analysis of the model. Another example is the one dimensional $1/r^2$ Ising model. For $\varepsilon > 0$, models with $J_{ij} = |i-j|^{-2+\varepsilon}$ were known to undergo a transition, those with $J_{ij} = |i-j|^{-2-\varepsilon}$ were known not to. What about the case $\varepsilon = 0$? This was important in the analysis of the Kondo problem [17] and the Thouless effect [18]. A rigorous argument [19] has recently settled this question, there is a phase transition for $\varepsilon = 0$. From these considerations we may formulate a philosophy about these methods. It is important to have an intuitive feeling for the properties of your model and desirable to have approximation schemes, especially simple approximation schemes, to get a rough feeling for the numbers of the model. It would be great to have exact solutions and we shall try to get as many of these as we can [20]. Barring exact solutions, it is very handy to know what is rigorously true about the model, especially if this proves simple to calculate.

Rigorous results provide a guidepost to further analyses and help choose between plausible and correct arguments and plausible and incorrect arguments. We turn now to the rigorous study of spin systems.

I.3 Second Analyses: Rigorous Results

As an illustration of the pitfalls which await the unwary, consider

$$m_1 = \lim_{|\Lambda|\to\infty} \lim_{h\to 0^+} \langle s \rangle_{\beta,h,\Lambda}$$

and

$$m_2 = \lim_{h\to 0^+} \lim_{|\Lambda|\to\infty} \langle s \rangle_{\beta,h,\Lambda}$$

for the two dimensional nearest neighbor Ising model on a lattice with free boundary conditions. The only difference is a change of order in the limiting operations, but that is sufficient for high β to make $m_1 = 0$ and $m_2 > 0$. Rigor is not only nice in these problems, it is demanded.

It is impossible to list here all the rigorous results known about spin systems; instead we include selected types of questions asked and known results. See [21] for discussions of rigorous results and the methods of proof involved. The first question that needed to be answered was, does the thermodynamic limit exist as a mathematical limit? We know that the pressure, defined as

$$p = \lim_{|\Lambda|\to\infty} \frac{1}{|\Lambda|} \ln Z_\Lambda$$

exists for many models. More importantly the correlation functions, which are the observables, are also known to exist. A simple proof of the existence of the spontaneous magnetization using plus boundary conditions may be made using the two correlation inequalities GKS I and GKS II. GKS I tells us that the spontaneous magnetization must be non-negative for all lattices, and GKS II tells us that the spontaneous magnetization is decreasing as a function of increasing lattice size. A monotone, bounded sequence must have a limit and so the spontaneous magnetization exists. Correlation inequalities relate the values of various expectation functions and are useful in arguments like the one above. Some of these are conveniently sequenced as Ursell functions ($\{\mathcal{U}_n\}$), i.e.,

$$\langle s \rangle \geq 0$$

is the first Ursell function $\mathcal{U}_1$, obeying GKS I.

$$\langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle \geq 0$$

is the second Ursell function $\mathcal{U}_2$, obeying GKS II.

$$\langle s_i s_j s_k \rangle - \langle s_i \rangle \langle s_j s_k \rangle - \langle s_j \rangle \langle s_k s_i \rangle$$
$$\langle s_i \rangle \langle s_j s_k \rangle - 2 \langle s_i \rangle \langle s_j \rangle \langle s_k \rangle \leq 0$$

is the third Ursell function $\mathcal{U}_3$, obeying the GHS inequality.

There are also others such as Newman's Gaussian inequality, the Lebowitz inequality and the FKG (Fortuin, Kastelyn, and Ginibre) inequality. Other lines of inquiry include the nature of thermodynamic states, the phase diagram of states and rigorous relations between critical exponents.

In this thesis we will study what is rigorously known about the transition temperature and the magnetization function. Results to date include upper and lower bounds on the transition temperature, upper bounds on the magnetization as a function of the temperature and the external field, and a lower bound on the spontaneous magnetization as a function of temperature (from the Peierls argument). It is clear that the transition temperature of any approximating model giving an upper bound on the magnetization automatically gives an upper bound on the true transition temperature. We should remark that there are two *a* *priori* different transitions possible in all these systems and hence two possible critical temperatures. One transition is the onset of spontaneous magnetization and this is the one we will use. The other transition is the loss of exponential falloff of the two point correlation function. While we believe these two transitions to occur at the same temperature for most of our models, the two dimensional x - y model is an example of a model where the two temperatures are distinct. Simon's inequality [22] provides a bound on this latter critical temperature. Applications of Simon's inequality to find numerical bounds of transition temperatures may be found in Barrett and O'Carroll [23] and Monroe [24].

Work on critical temperature bounds began with Peierls and the lower bound on T_c he derives from the Peierls argument. In 1976 Jurg Frohlich, Barry Simon and Tom Spencer [25] discovered the infrared bounds which gave (relatively) easy to compute lower bounds for n - vector models. These are the two methods we have for computing lower bounds. Griffiths first proposed an argument to give an upper bound on T_c for spin $1/2$ models. His bound is slightly better than the mean field critical temperature. Cassandro, Olivetti, Pellegrinotti and Presutti [26] used a result in probability called Dobrushin's Uniqueness Theorem [27] to extend the mean field upper bound to a large class of one - component models, including the spin $n/2$ models, thus extending the bound to more than spin $1/2$ models. Driessler, Landau and Perez [28] and Simon [29] were able to extend this bound to multicomponent, i.e. n-vector, models. Fisher [30] concentrated on nearest neighbor models. By using self avoiding walk ideas he was able to get the strongest bounds that we have on such models. A table of all these bounds is given in figure 4.

The magnetization function first received attention from Thompson [31]. He showed that the mean field magnetization was a bound on the true magnetization for spin $1/2$ models. This implies the mean field critical temperature bound.

Krinsky [32] narrowed the scope of Thompson's work to nearest neighbor models and was able to show that the Bethe approximation gave an upper bound to the magnetization. The Bethe approximation is one of the Cluster Variational approximations and constitutes the strongest result presently known for nearest neighbor spin $1/2$ magnetization and temperature bounds. The approximation itself will be described in chapter II. By different methods, the mean field magnetization was extended to spin $n/2$ and multicomponent models. Paul Pearce [33] used techniques similar to those used in correlation inequality proofs to get the mean field bound for spin $n/2$ models (where $n = 2^p 3^q - 1$, p and q are non-negative integers and not both zero), and the x - y and classical Heisenberg models. Hal Tasaki and Takashi Hara [34] use correlation inequalities to demonstrate the bound for spin $n/2$, n any positive integer, and n-vector models where $n \geq 3$. Combining Pearce's work and Tasaki and Hara's work we have the mean field bound for all spin $n/2$ and all n-vector models. Joseph Slawny [35] uses the DLR (Dobrushin, Lanford and Ruelle) equations and a new inequality analogous to Jensen's inequality to independently arrive at the mean field bound for all spin $n/2$ and all n-vector models. We should also mention Charles Newman [36] who has results similar to Tasaki and Hara's. Pearce's and Slawny's work will be discussed in Sections IV and V, respectively.

Our new result is a proof of bounds on the true magnetization by the second and third members of the Cluster Variational approximations, the Oguchi method and (where appropriate) the three body approximation. These bounds hold for general ferromagnetic pair coupling, not necessarily nearest neighbor couplings, for spin $1/2$ Ising models. The resulting critical temperature bounds are also shown to be a decreasing sequence,

$$T_C(\text{true}) \leq T_C(\text{symmetric 3--body}) \leq T_C(\text{Oguchi}) \leq T_C(\text{mean field})$$

as expected. When the couplings in the privileged regions for each of these approximations are non-zero, the temperature bounds are shown to be strict.

In the next chapters we will review Pearce's work and Slawny's work and then present our new bounds. We shall focus attention to one component models, mainly spin $n/2$.

Chapter II
Mean Field Theory and Extensions

II.1 Mean Field Theory

Since mean field theory will be the basis for the bounds we will derive in the following chapters, it is good to get an intuitive picture of what is happening. We believe that in the thermodynamic limit we will have some unique equilibrium state. In this state we expect each site to have the same average value or (in other words) the magnetization should be uniform throughout the (infinite) lattice. If this is so, we may make a self consistency argument to discover the value of that magnetization. This argument was first given by Pierre Weiss in 1907. Instead of performing the full configurational average, we concentrate attention on one spin. We replace all other spins by their assumed average value m. Thus our Hamiltonian (equation I.1) has become

$$\mathrm{H}_1 = -\sum_{j\neq i} J_{ij} s_i m - h\sum_{j\neq i} m - hs_i \tag{II.1}$$

where s_i is the spin we are looking at. We now drop the subscript 'i' since we have only one variable. This new lattice creates a background field for our spin s through the pair couplings and we can compute the predicted magnetization of spin s in the usual fashion,

$$\langle s \rangle_{\beta,\mathrm{H}_1} = \frac{\left[\sum_{s\varepsilon\Omega} s e^{-\beta \mathrm{H}_1}\right]}{\left[\sum_{s\varepsilon\Omega} e^{-\beta \mathrm{H}_1}\right]} \tag{II.2}$$

Now we had originally assumed that all the spins were equivalent, hence we demand that this procedure yield the value m for the expectation of our 'privileged' spin. This will give us a self - consistent theory with the assumptions we've made. The consistency equation is then

$$m(\beta) = \langle s \rangle_{\beta,\mathbf{H}_1}$$

For the spin $1/2$ model this gives the familiar equation

$$m = \tanh(\beta \sum_j J_{ij} m + h) \qquad \text{(II.3)}$$

whose largest root is our estimate at the true magnetization (using the Hamiltonian given in equation I.1).

A few comments are in order about rigorously using this procedure. First, of necessity we start our calculation in a finite region Λ that later we expand to the thermodynamic limit. If we use translation invariant couplings on a lattice with periodic boundary conditions and a sequence of intermediate lattices, such as cubes, where all sites are equivalent, we will have translation invariant finite lattice states. The thermodynamic limit will also then be translation invariant and our assumption about equivalent sites will be correct. Second, we observe that if $m(\beta)$ is a bound on the expectation of the spin, then any function $m^*(\beta)$, with $m^*(\beta) \geq m(\beta)$, is also a bound. The best bound for a given Λ will be the (pointwise) smallest function that is a bound. We anticipate the Λ dependence of this best bound, call it $m_\Lambda(\beta)$, and note that inspection of the form of $m_\Lambda(\beta)$, from say equation II.2, reveals that it is an increasing function of $|\Lambda|$. It will also be bounded above by the infinite volume magnetization bound and will approach this as a limit. The infinite volume magnetization bound is what we will call the magnetization bound. Third, the constant term in the Hamiltonian $\mathbf{H}_1$ may be thrown away when considering expectation values. We note that $\mathbf{H}_1$ is now a function of only one spin variable and the configurational sum is now easy. Our extensions to mean field theory will also get rid of a large number of spins and leave Hamiltonians that are functions of only a small, easy to work with, number of spins. Fourth, the equation II.3 is usually solved graphically. A plot of m and an overlaid plot of $\tanh(\beta \sum_j J_{ij} m + h)$ as functions of m will quickly yield an estimate of the intersection value. Further numerical work, such as Newton's method for finding zeroes of functions, will give better and better estimates of the intersection value. Figure 5 shows this graph. Fifth, the critical temperature is the maximum temperature (minimum β) such that equation II.3 has a non - zero solution for $h = 0$. Taking derivatives of equation II.3 we see that this occurs at

$$\beta_c \sum_j J_{ij} = 1$$

or

$$T_c = \sum_j J_{ij}$$

The general condition for the critical temperature from equation II.5 is

$$\left. \frac{\partial \langle s \rangle_{\beta, \mathrm{H}_n(m)}}{\partial m} \right|_{m=0} = 1 \qquad \text{(II.4)}$$

and this equation also defines the critical temperatures of the extensions to mean field theory.

Mean field theory is also known as the Curie - Weiss effective field theory. The self consistency idea and procedure are also used in the Hartree Fock approximation, used to find an approximate wave function describing a system of many electrons.

II.2 Extended Mean Field Theories

The extensions to mean field theory that we describe here use the same self - consistency idea. The philosophy behind these extensions is that while an infinite number of spin variables (needed for the full configurational sum) may be unmanageable, and one spin variable used in mean field theory may be fine for a first approximation, some procedure should exist by which with more and more calculational effort a better and better guess to the true magnetization will be obtainable. The cluster variational approximations are a procedure that fulfills this need. Intuitively these approximations are reasonable, yet only the first cluster variational approximation, i.e., mean field theory, has been shown to be a bound for most spin systems. For spin $1/2$ systems, this thesis shows that the next two approximations, the Oguchi approximation and (where appropriate) the three body approximation, are also magnetization bounds. A stronger approximation has been shown to be an upper bound for the special case of spin $1/2$ systems with only nearest neighbor couplings. This stronger bound is the Bethe approximation [32] (also called the Bethe-Peierls-Weiss or BPW approximation).

The procedure for these higher order approximations is for the n'th order approximations to look at n selected spins in Λ. All other spins are replaced by their assumed magnetization m. The interactions between the n spins themselves and between the n spins and the background field are kept unchanged. The calculation of the expectation values of each of these spins is done exactly using the effective Hamiltonian. If we call X the region containing the privileged spins, the effective Hamiltonian H_n is

$$\mathrm{H}_n = -\frac{1}{2}\sum_{i,j\varepsilon X} J_{ij} s_i s_j - \sum_{i\varepsilon X, j\varepsilon \Lambda\setminus X} J_{ij} s_i m - h\sum_{i\varepsilon X} s_i$$

This may be written in the simpler form:

$$\mathrm{H}_n = -\frac{1}{2}\sum_{i,j\varepsilon X} J_{ij} s_i s_j - \sum_{i\varepsilon X}(h + J_i(X)m)s_i$$

where

$$J_i(X) = \sum_{j\varepsilon\Lambda\setminus X} J_{ij}$$

If $\langle s_i \rangle_{\beta,\mathrm{H}_n}$ is independent of 'i' , the magnetization is taken to be the largest self - consistent solution m of

$$m = \langle s_i \rangle_{\beta, \mathbf{H}_n} \tag{II.5}$$

The Oguchi bound corresponds to selecting any two spins. In practice these are chosen to be nearest neighbors since these spins usually have the strongest spin-spin coupling. If our region $X = \{s, t\}$ with coupling J, the Oguchi Hamiltonian is

$$\mathbf{H}_2 = -Jst - k(s+t) \tag{II.6}$$

where

$$k = h + J_i(X)m$$

(We will often use the mixed notation $X = \{s, t\}$ instead of $X = \{i, j\}$ and $s \equiv s_i$ and $t \equiv s_j$. What is meant should be clear from context.) The three body approximation considers any three spins. If our region is $X = \{s, t, u\}$, the three body Hamiltonian $\mathbf{H}_3$ is

$$\mathbf{H}_3 = -J_{st}st - J_{su}su - J_{tu}tu - k_s(X)s - k_t(X)t - k_u(X)u \tag{II.7}$$

where J_{xy} is the coupling between spins x and y, and $k_y(X) = h + J_y(X)m$. In the Bethe approximation we will look at a spin and all of its (assumed) equivalent nearest neighbors. The magnetizations of the central spin and the external spins are calculated in the background field as before. However our new self consistency condition is

$$\langle s_{central} \rangle = \langle s_{nearest\ neighbor} \rangle .$$

Where applicable, the Bethe approximation has yielded the strongest magnetization and critical temperature bounds to date.

Chapter III

The Models: Mathematical Summary

Let Λ be a finite lattice with periodic boundary conditions. At each site 'i' in Λ there is a spin variable s_i taking values in the spin space Ω_i with weights $d\mu_i(s)$. The configuration space for Λ is $\bigotimes_{i\varepsilon\Lambda}\Omega_i$, written as $[s]$, with *a priori* measure $\bigotimes_{i\varepsilon\Lambda} d\mu_i(s)$. The Ω_i and $d\mu_i(s)$ are usually identical copies of one basic Ω and $d\mu(s)$. Spin $n/2$ spins have

$$\Omega = \{-1\ ,\ -1+\frac{2}{n}\ ,\ -1+\frac{4}{n}\ ,\ \cdots\ 1\}$$

with the associated normalized counting measure. Our interactions are defined through the Hamiltonian

$$\mathrm{H} = -\frac{1}{2}\sum_{i,j\varepsilon\Lambda} J_{ij}s_i s_j - h\sum_{i\varepsilon\Lambda} s_i$$

where $J_{ij} \geq 0$ and $h \geq 0$ are ferromagnetic couplings and $J_{ij} = J(|i-j|)$ is translation invariant. We assume $\sum_j J_{ij}$ is finite and use the convention that $J_{ii} = 0$. $\beta = 1/kT$ is the inverse temperature and we define expectations via the usual Boltzmann factor,

$$\langle f\rangle_{\Lambda,\mathrm{H}} = \frac{\left(\sum_{[s]} f e^{-\beta\mathrm{H}}\right)}{\left(\sum_{[s]} e^{-\beta\mathrm{H}}\right)}$$

β will usually be absorbed into the couplings J_{ij} and h. The magnetization of the model is defined as

$$\langle s_i\rangle = \lim_{|\Lambda|\to\infty}\langle s_i\rangle_\Lambda$$

and the spontaneous magnetization is

$$m = \lim_{h\to 0^+}\langle s_i\rangle$$

Our states are translation invariant so both of the preceding equations are actually site independent. By general results, this spontaneous magnetization is the same as that obtained by plus boundary conditions (see chapter I.1 for a discussion of boundary conditions). When the underlying lattice is $\mathbb{Z}^d$, our approach to the thermodynamic limit will be through a sequence of nested cubes.

We will refer to several correlation inequalities repeatedly and we list them here for reference:

Correlation Inequalities	
Name [Reference]	Inequality
GKS I [37]	$\langle s \rangle \geq 0$
GKS II [38]	$\langle st \rangle - \langle s \rangle\langle t \rangle \geq 0$
GHS [39]	$\langle stu \rangle - \langle s \rangle\langle tu \rangle - \langle t \rangle\langle su \rangle$
	$- \langle u \rangle\langle st \rangle + 2\langle s \rangle\langle t \rangle\langle u \rangle \geq 0$
FKG [40]	$\langle fg \rangle - \langle f \rangle\langle g \rangle \geq 0$

where s, t, u are spin variables associated with (possibly) different sites and f, g are monotone functions of spin variables. By a monotone function we mean any function that does not decrease as any of its arguments increase. Examples of monotone functions include s and $\sum_i s_i$.

When working with mean field theory or its extensions, we shall often consider regions X_α, all identical copies of some region X, such that $\Lambda = \bigcup_\alpha X_\alpha$, i.e., Λ is a disjoint union of the basic region X and its copies. We denote

$$J_i(X) = \sum_{j \in \Lambda \setminus X} J_{ij}$$

for any site i in some copy of X. Often the mixed notation $X = \{s, t\}$ will be used instead of $X = \{i,j\}$ and $s \equiv s_i$ and $t \equiv s_j$ when it is clear what is meant. J_{st} will stand for J_{ij} if $s = s_i$ and $t = s_j$, k ($\equiv k(m)$) will be short for $h + \sum_j J_{ij} m$ and $k_i(X)$ will stand for $h + J_i(X)m$. Similarly k_s and $J_s(X)$ refer to k_i and $J_i(X)$ when $s = s_i$. The variables s, t, u, x and y will often be used for spin variables instead of s_i, s_j, etc. m will always refer to a magnetization. α, β and γ used as exponents will be binary variables assuming only the values 0 and 1. The relational symbol $\sim$ will stand for 'has the sign of' , where zero is taken to be either positive or negative as is convenient. For example $\sim(-)^\alpha$ means has the sign of $(-1)^\alpha$. Non-negativity is also written $\sim(+)$.

We will use ■ to indicate the end of a proof.

Chapter IV

Pearce: Re-examining the Mean Field Magnetization Bound

IV.1 The Pearce Results

Pearce's work extends the mean field magnetization bound of Thompson in two ways. First, the method of proof used is simpler and more adaptable to proofs of other results. Second, the mean field bound is shown to apply to more than spin $1/2$ models, it also applies to spin $n/2$ models (where $n = 2^p 3^q - 1$, p, q are non-negative integers and not both zero), the x - y model, and the classical Heisenberg model.

The method of proof is quite similar to the methods used in proving the correlation inequalities GKS I and GKS II. There one makes several variable changes, expands the exponential and notices that what is left may be factored over sites. The resulting expression is a one or two variable polynomial inequality which can be directly proven. Retracing these steps gives one the correlation inequality for any finite volume, and hence for the infinite volume limit. These proofs are written out in Appendix A. Pearce will show $\langle m - s \rangle \geq 0$ where m is the mean field magnetization. To do this we follow the above procedure until we arrive at a simple one - variable inequality (equation IV.1). This is theorem IV.1. For two single spin measures, spin $1/2$ and spin 1, we are able to demonstrate equation IV.1 by a variety of methods. This is theorem IV.2. We then notice that a convolution theorem enables us to infer equation IV.1 for the spin $n/2$ measures mentioned above. This will be theorem IV.3. Some numerical investigation of equation IV.1 was done in hopes of illuminating how to categorize the class of measures satisfying equation IV.1. While equation IV.1 was found to be true in all cases tested, no systematic properties of the equation were revealed.

In this proof we use periodic boundary conditions. We refer the reader to chapter III for the necessary mathematical assumptions and notation and to chapter II.1 for the argument concerning passage to the thermodynamic limit. We write m for $m(\beta,\Lambda)$ and for notational convenience suppress the dependence on β and Λ. We remark that k in equation IV.1 is short for $h + m\sum_{j\neq i} J_{ij}$, which is the coefficient of the spin s obtained from the Hamiltonian H_1 (equation II.1). This specific form of k will be important in the interpretation of m as the mean field magnetization, however only the positivity of k is needed in the proofs of all the theorems. The ideas and most of the results of the following are from Pearce [45].

Theorem IV.1 : Given a spin space Ω, associated measure $d\mu(s)_\Lambda$ and a constant m satisfying Pearce's Inequality:

$$\int e^{ks}(m-s)^p \, d\mu(s) \geq 0 \tag{IV.1}$$

for all non - negative integral p, we have

$$m \geq \langle s \rangle_{\mathrm{H}}$$

Proof : If $\langle (m-s) \rangle \geq 0$ we have the result. We examine the Hamiltonian (equation I.1) and note it can be rewritten as:

$$\mathrm{H} = -\frac{1}{2}\sum_{i,j} J_{ij} \left[(m-s_i)(m-s_j) + m(s_i+s_j) - m^2 \right]$$

so that

$$\langle (m-s) \rangle_{\mathrm{H}} = \mathrm{N}^{-1} \langle (m-s) \exp(\frac{1}{2}\sum_{i,j} \beta J_{ij}(m-s_i)(m-s_j)) \rangle_{\beta,\mathrm{H}_0} \tag{IV.2}$$

where $\mathrm{H}_0 = \sum_{i\varepsilon\Lambda} \mathrm{H}_1(s_i)$, H_1 defined in equation II.1, and

$$\mathrm{N} = \langle \exp(\frac{1}{2}\sum_{i,j} \beta J_{ij}(m-s_i)(m-s_j)) \rangle_{\beta,\mathrm{H}_1}$$

We are only interested in the non - negativity of $\langle (m - s) \rangle$ so we may neglect all positive terms on the right hand side of equation IV.g., **N** is clearly positive. We expand the exponential into a Taylor's series and write out some terms of the numerator (NUM):

$$NUM = \langle (m-s) \prod_{i,j} (\sum_{n=0}^{\infty} \frac{1}{n!} \left[\frac{1}{2} \beta J_{ij} (m-s_i)(m-s_j) \right]^n) \rangle_{\beta,\mathbf{H}_1}$$

Observe that the resulting expression is a sum of terms like

$$(positive\ \ coefficient) \langle \prod_i (m-s_i)^{p_i} \rangle_{\beta,\mathbf{H}_0}$$

Since $\mathbf{H}_0$ is a sum of one - variable terms, each of these terms is

$$(positive\ \ coefficient) \prod_i \langle (m-s_i)^{p_i} \rangle_{\beta,\mathbf{H}_1}$$

(Note the change of order of operations of expectation and continued product.) Our hypothesis implies that $\langle (m-s_i)^{p_i} \rangle_{\beta,\mathbf{H}_1}$ is non - negative, so that $\langle (m-s) \rangle_{\mathbf{H}}$ is a sum of terms, each of which is a product of non - negative terms, hence $\langle (m-s) \rangle_{\mathbf{H}}$ is non - negative. ▪

We observe that for even p equation IV.1 is obviously positive. We consider now only odd p. For two measures, spin $1/2$ and spin 1 we can show equation IV.1 directly.

Theorem IV.2 If m is defined by demanding that equation IV.1 is identically zero for $p = 1$, then equation IV.1 holds for the spin $1/2$ and spin 1 measures.

Proof : The spin $1/2$ measure is:

$$d\mu(s) = \frac{1}{2} \{ \delta(s+1) + \delta(s-1) \}$$

The value of m, after algebraically manipulating equation IV.1 is

$$m = \frac{\int e^{ks} s\, d\mu(s)}{\int e^{ks} d\mu(s)}$$

or

$$m = \tanh k$$

Equation IV.1 for odd p is

$$e^{-k}(1+\tanh k)^p - e^k(1-\tanh k)^p \geq 0$$

Some algebra reduces this to

$$e^{k(p-1)} - e^{k(1-p)} \geq 0$$

which is clearly true for p odd and k positive.

The spin 1 measure is

$$d\mu(s) = \frac{1}{3}(\delta(s+1) + \delta(s) + \delta(s-1))$$

The expression for m is now

$$m = (e^k - e^{-k})/(e^k + 1 + e^{-k})$$

Equation IV.1 for odd p is:

$$\frac{1}{e^k + 1 + e^{-k}}\left[e^{-k}(2e^k + 1)^p + (e^k - e^{-k})^p - e^k(2e^{-k} + 1)^p\right] \geq 0$$

For $p = 1$ equality holds (by definition). For $p \geq 3$,

$$(2e^k + 1)^p \geq (2e^k + 1)^2(2e^{-k} + 1)^{p-2}$$

so the expression in brackets is

$$(e^k - e^{-k})^p + (2e^{-k} + 1)^{p-2}(4e^k + 4 + e^{-k} - 4e^{-k} - 4 - e^k)$$

$$= (e^k - e^{-k})^p + (2e^k + 1)^{p-2}(3)(e^k - e^{-k})$$

which is non - negative. ■

Direct manipulation of equation IV.1 gets progressively more difficult with higher spin $n/2$ measures. Note that once equation IV.1 has been proven for $d\mu(s)$, it has also been proven for $\alpha d\mu(\beta s)$ with α and β any positive constants. We use this fact to write higher spin $n/2$ measures as convolutions of spin $m/2$ and spin $q/2$ measures where

$$(n+1) = (m+1)(q+1)$$

Rewriting equation IV.1 in terms of the related generating function allows us to use the convolution property to infer equation IV.1 for higher spin $n/2$ measures.

Theorem IV.3: Equation IV.1 holds for spin $n/2$ measures where $n = 2^p 3^q - 1$ where p and q are non - negative integers and not both zero.

We introduce the convolution

$$d(\mu_1 * \mu_2)(s) = \int d\mu_1(t) d\mu_2(s-t).$$

For example, a spin $3/2$ measure may be written as a convolution of two modified spin $1/2$ measures by

$$d\mu(x) = \int \frac{1}{2}\left[\delta(x-s+\frac{1}{3}) + \delta(x-s-\frac{1}{3})\right]\frac{1}{2}\left[\delta(s+\frac{2}{3}) + \delta(s-\frac{2}{3})\right]ds$$

<u>Proof</u> : Consider the generating function $g(\mu,x)$ related to equation IV.1.

$$g(\mu,x) = \sum_{p=0}^{\infty} \int e^{ks}(m-s)^p x^p \frac{1}{p!} d\mu(s) \qquad \text{(IV.3)}$$

$$= \int \exp\left[(k-x)s + mx\right] d\mu(s)$$

Non - negativity of equation IV.1 is equivalent to non - negativity of the coefficients of $g(x)$ expanded in a Maclaurin series. If we write

$$\varphi(\mu,k) = \int e^{ks} d\mu(s)$$

and

$$D(\mu,k) = \log\varphi$$

then equation IV.3 is

$$g(\mu,x) = \exp\left[D(\mu,k-x) + x\frac{d}{dk}D(\mu,k)\right]$$

Under convolution,

$$D(\mu_1 * \mu_2,k) = D(\mu_1,k) + D(\mu_2,k)$$

so

$$g(\mu_1 * \mu_2,x) = g(\mu_1,x)g(\mu_2,x)$$

which implies non - negativity of the coefficients of $g(\mu_1 * \mu_2,x)$ given the same information about $g(\mu_1,x)$ and $g(\mu_2,x)$. Since we have directly shown the truth of equation IV.1 for spin $1/2$ and spin 1 , we now know that equation IV.1 holds for any measure expressible as a convolution of these two measures. This is the class of measures listed in the statement of the theorem. As a limiting case, we have shown that the spin - ∞ measure, $d\mu(s) = \frac{1}{2}ds$ is one for which the mean field bound holds. For this model, equation IV.1 is

$$m = L(\sum_j J_{ij} m + h)$$

where $L = \coth x - \frac{1}{x}$ is the Langevin function. ▪

IV.2 Analyses of the Pearce Inequality

It is interesting to try to classify the measures $d\mu(s)$ such that equation IV.1 holds. Attempts in this direction have resulted in an alternative proof of Theorem IV.2 for spin $1/2$ measures; a proof of Theorem IV.2 for a portion of the k,n plane; and a proof of Theorem IV.2 for various values of m. Numerical investigation of Pearce's equation IV.1 has not resulted in any counterexamples. These results are examined below.

We must remark that although the validity of equation IV.1 for all spin $n/2$ measures is still an open question and therefore an interesting one to continue to investigate, there is no longer any statistical mechanical interest in this problem. The interest in equation IV.1 lay in its role as a stepping stone to proving the mean field magnetization bound. By different methods Slawny has already proven the mean field bound for a large class of measures that includes the spin $n/2$ measures.

Spin 1/2

We consider first spin $1/2$. A geometric picture of the problem is made by an analogy to a seesaw. We divide the interval $[-1\ ,\ 1]$ into two segments $[-1,m)$ and $[m,1]$ and attach weights (also known as mass points) e^{-k} to the end of the left segment and e^{k} to the end of the right segment. (See figure 6.) Equation IV.1 may be viewed as a statement about torques. For $p = 1$, the torques balance, i.e.,

$$e^{-k}(1+m) = e^{k}(1-m) \tag{IV.4}$$

Other seesaw arrangements, with lever arms of $(1+m)^p$ and $(1-m)^p$ presumably don't balance, i.e., equation IV.1 states

$$e^{-k}(1+m)^p \geq e^{k}(1-m)^p \tag{IV.5}$$

We see this directly from equation IV.4 since

$$e^{-k}\frac{(1+m)}{(1-m)} = e^{k}$$

and

$$\frac{(1+m)}{(1-m)} \geq 1 \quad \rightarrow \quad \left[\frac{(1+m)}{(1-m)}\right]^{p} \geq \frac{(1+m)}{(1-m)}$$

so we've shown equation IV.5. This constitutes an alternative derivation of Theorem IV.2 for spin $1/2$.

Hölder's Inequality

Examination of the above proof shows that one does not need the explicit exponential form for the weights, only that the weight on the right be greater than the weight on the left. Let us generalize our problem to a compound torque problem, this will correspond to spin $n/2$ measures. We will have a set of weights on the left of the balance $w_{i,L}$, at a set of distances $d_{i,L}$. Similarly on the right we have a (different) set of weights $w_{j,R}$, at distances $d_{j,R}$. The number of weights on both sides do not have to be equal. Clearly the correspondence of this formulation to our original problem is

$$\{w_{j,R}\} = \{e^{kx} \;\mid\; x \,\varepsilon\, \Omega \text{ and } x > m\}$$

$$\{w_{i,L}\} = \{e^{kx} \;\mid\; x \,\varepsilon\, \Omega \text{ and } x < m\}$$

$$\{d_{j,R}\} = \{x - m \;\mid\; x \,\varepsilon\, \Omega \text{ and } x > m\}$$

$$\{d_{i,L}\} = \{m - x \;\mid\; x \,\varepsilon\, \Omega \text{ and } x < m\}$$

If the mean m lies exactly on a point in Ω, this point will not contribute to equation IV.1 and also clearly does not contribute to our torque problem since the extra weight falls directly on the balance point. The definition of the balance point m (mean and magnetization) is

$$\sum_i w_{i,L} d_{i,L} = \sum_j w_{j,R} d_{j,R}$$

Equation IV.1 asks us to determine the sign of

$$\sum_i w_{i,L} d_{i,L}^p - \sum_j w_{j,R} d_{j,R}^p \sim \frac{\sum_i w_{i,L} d_{i,L}^p - \sum_j w_{j,R} d_{j,R}^p}{\sum_i w_{i,L}}$$

$$\geq \left[\sum_i \frac{w_{i,L}}{\sum_i w_{i,L}} d_{i,L} \right]^p - \sum_j \frac{w_{j,R}}{\sum_i w_{i,L}} d_{j,R}^p$$

(Hölder's Inequality)

$$= \left[\sum_j \frac{w_{j,R}}{\sum_i w_{i,L}} d_{j,R} \right]^p - \sum_j \frac{w_{j,R}}{\sum_i w_{i,L}} d_{j,R}^p \qquad \text{(IV.6)}$$

Expand the first term. Looking only at the coefficients of $d_{j,R}^p$, we see that if

$$\left[\frac{w_{j,R}}{\sum_i w_{i,L}} \right]^p \geq \frac{w_{j,R}}{\sum_i w_{i,L}} \qquad \text{(IV.7)}$$

then equation IV.6 is positive. Equation IV.7 is true if

$$w_{j,R} \geq \sum_i w_{i,L}$$

for each $w_{j,R}$. For Pearce's equation, we evaluate $\sum_i w_{i,L}$ explicitly and use the smallest value of $w_{j,R}$ we can. Since the weights are a geometric series, if we let c be the common ratio between adjacent weights, and if there are M of them, we ask:

$$c^{M+1} \geq 1 + c + \cdots c^M$$

which holds for all M if $c \geq 2$. In terms of Pearce's weights, a sufficient condition is then

$$e^{2k/n} \geq 2$$

or

$$k \geq \frac{n \ln 2}{2}.$$

What we have shown is that for any spin $n/2$ measure, if the external field is strong enough, the mean field magnetization will be a bound on the true magnetization.

Geometric Analysis

We may also investigate Pearce's problem geometrically. For the spin $1/2$ case, we note that there is a hyperbola indicating the possible pairs of values $(d_{i,L}, w_{i,L})$ that leave the position of the mean unchanged. From our previous analysis, any such pair with $d_{i,L} > d_{j,R}$ still obeys equation IV.1. We shall now construct a distribution of distances and weights so that it is obvious that

$$\sum_i w_{i,L} d_{i,L}^p - \sum_j w_{j,R} d_{j,R}^p \geq 0$$

Choose any set of values for $d_{j,R}$ and $w_{j,R}$. Let $\{d_{i,L}\}$ be the same set of values as $\{d_{j,R}\}$ and similarly for $\{w_{i,L}\}$. This is geometrically equivalent to reflecting the right hand side distribution through a mirror located at the balance point and perpendicular to our line segment $[-1,1]$. Now take any pair $(d_{i,L}, w_{i,L})$ and substitute for it the pairs $(d_{i,L}, \alpha w_{i,L})$ and $(d_{i,L}^*, \frac{d_{i,L}}{d_{i,L}^*}(1-\alpha) w_{i,L})$ where $0 \leq \alpha \leq 1$ and $d_{i,L}^* > d_{i,L}$. The balance point is undisturbed since

$$d_{i,L} w_{i,L} = d_{i,L} \alpha w_{i,L} + d_{i,L}^* \left(\frac{d_{i,L}}{d_{i,L}^*} (1-\alpha) w_{i,L} \right)$$

What we have done is to take part of the weight associated with $d_{i,L}$ and shift it to some distance $d_{i,L}^*$ farther away from the balance point. In the spin $1/2$ case we shifted all of the weight associated with the initial pair $(d_{i,L}, w_{i,L})$. See figure 7. This shifting process leaves the balance point unchanged yet increases the value of $\sum_i w_{i,L} d^p_{i,L}$ since it effectively lets the process of raising a number to a power p work on a greater number. Thus for any distribution constructible in this manner,

$$\sum_i w_{i,L} d^p_{i,L} \geq \sum_j w_{j,R} d^p_{j,R}$$

which is what we wanted to show.

How do we use this geometrically proven inequality to analyze Pearce's inequality? When the initial distribution gives a set of distances and weights such that the final distribution may be obtained only by decreasing the initial weights in the hyperbolic manner described, then the final distribution will satisfy the Pearce inequality. One case we know is constructible is one where

$$\{d_{i,L}\}_{initial} \subseteq \{d_{i,L}\}_{final}$$

and the remaining members of $\{d_{i,L}\}_{final} \setminus \{d_{i,L}\}_{initial}$ are farther out than any element of $\{d_{i,L}\}_{initial}$. The proof of constructibility is by contradiction. Start with the initial distribution and redistribute weights, making sure that first the weight associated with the smallest distance is correct for the final distribution and working your way to greater and greater distances (farther and farther out from the balance point). When you have no more excess weights to work with, can this distribution be any different from the final distribution? If it is, then one of the two distributions has extra weights on the left hand side. But this contradicts the fact that both distributions have the same balance point and the same right hand side torques. Thus the two distributions must be equal and you have constructed the distribution you wanted to prove the Pearce inequality for.

Notice that the spin values $\{x_i \mid x_i \varepsilon \Omega\}$ are regularly spaced and that the weights e^{kx_i} are increasing. If the mean m happens to lie exactly on a point in Ω, or midway between two adjacent points in Ω we have an obviously constructible distribution by the previous argument. Thus if $m \varepsilon \{0, \frac{1}{N}, \cdots 1\}$, Pearce's inequality holds. When $\Omega = [-1,1]$, m must lie on a point in Ω and so whenever the distribution of weights is non - decreasing, e.g., the spin ∞ distribution, Pearce's inequality must hold. This is a proof of Pearce's Lemma 4, stated below:

> Let μ be an even probability measure with support on $[-1,1]$, and suppose μ is absolutely continuous, i.e., $d\mu(s)=f(s)ds$, with f non-decreasing on $[0,1]$. Then equation IV.1 holds for this measure.

In fact our analysis is slightly stronger than Pearce's Lemma 4 in that given knowledge of the range of values of m as some subset of $[0,1]$, we can relax the non - decreasing condition of the weights.

A variant of our proof that the spin $1/2$ model satisfies Pearce's inequality yields some information about spin $n/2$ systems. The greatest two values a spin $n/2$ spin can assume are $\frac{n-2}{n}$ and 1. Whenever $m \varepsilon [\frac{n-1}{n}, 1]$, we notice there is only one set of values in $\{d_{j,R}, w_{j,R}\}$ and

$$\sum_i w_{i,L} d_{i,L} = w_{j,R} d_{j,R}$$

But by our location of m, each $d_{i,L} \geq d_{j,R}$ so

$$\sum_i w_{i,L} d_{i,L}^p \geq w_{j,R} d_{j,R}^p$$

so Pearce's inequality holds. Except for the spin $1/2$ case, this is a weaker result than our (k,n) result. We summarize our results in the following

Theorem IV.4: For spin $n/2$, if $k \geq n\frac{\ln 2}{2}$ or $m \varepsilon \{0, \frac{1}{n}, \cdots \frac{n-2}{n}\} \cup [\frac{n-1}{n}, 1]$ then Pearce's inequality holds. If $d\mu(s) = f(s)ds$ and $f(s)$ is non-decreasing, Pearce's inequality holds.

Proof : Given Above. ▪

Numerical Analysis

A numerical investigation of the Pearce inequality was made in hopes of indicating where analytic proofs of the inequality should be directed. A listing of the program used, together with comments and instructions is in figure 8. The magnetization, usually a function of the external field, was allowed to vary independently for use in testing conjectures where the value of the magnetization was unimportant. No counterexamples were found, nor were any important properties of the equation revealed. Numerical examples are given in figure 9.

Chapter V

Slawny: Completing the Mean Field Analysis

V.1. Other Magnetization Bound Ideas

After Pearce's work in June 1980, it seemed extremely reasonable to assume that the mean field magnetization bound held for all spin $n/2$ measures; it only remained to be seen how to do so. Pearce's method proved to be a very 'bare handed' approach to analyzing the problem and further attempts at straightforwardly solving the Pearce inequality for more spin $n/2$ measures didn't work out. In December 1981 Charles Newman succeeded in proving the magnetization bound for one-component systems whose expectations obeyed the GHS (Griffiths, Hurst and Sherman) inequalities. The GHS inequalities are a set of inequalities expressing the multivariable analogue of a one - variable concavity property, i.e.,

$$\langle s_i s_j s_k \rangle - \langle s_i s_j \rangle\langle s_k \rangle - \langle s_i s_k \rangle\langle s_j \rangle - \langle s_j s_k \rangle\langle s_i \rangle + 2\langle s_i \rangle\langle s_j \rangle\langle s_k \rangle \leq 0 \qquad (V.1)$$

for all $i, j, k \, \varepsilon \Lambda$, not necessarily distinct. If we consider only one site, equation V.1 reduces to

$$\langle s^3 \rangle - 3\langle s^2 \rangle\langle s \rangle + 2\langle s \rangle^3 \leq 0$$

which is essentially

$$\frac{\partial^2 \langle s \rangle}{\partial k^2} \leq 0$$

or concavity. Since it had been proven that a large class of spin measures, including spin $n/2$, obeyed the GHS inequalities, Newman had succeeded in extending the magnetization bound. Newman's work went unpublished. About

November 1983 Hal Tasaki and Takashi Hara found their own proof of the magnetization bounds for single component spins obeying the GHS inequality. In addition, Tasaki and Hara extended Pearce's proof of the mean field bound to n - component systems with $n \geq 3$. Since Pearce had shown the bound for $n \leq 3$ multicomponent systems, this new result rounded out the domain of validity of the magnetization bound.

In March 1983 Joseph Slawny published a proof of the mean field bound using still different methods. His results are valid for a class of one component models which includes spin $n/2$, and for arbitrary n - component models. To explain the idea of his proof, we shall temporarily focus on the spin $1/2$ measure. Recall that the mean field magnetization is defined as the greatest self consistent solution of

$$m_{MF} = \tanh(m_{MF} \sum_j J_{ij} + h)$$

This is shown graphically in figure 10. (We absorb the β dependence into the couplings in this chapter.) If we can show that the true magnetization satisfies

$$m_{true} \leq \tanh(m_{true} \sum_j J_{ij} + h) \qquad \text{(V.2)}$$

then by inspection of figure 11 we see that $m_{true} \in [0, m_{MF}]$ so we've shown $m_{true} \leq m_{MF}$. To derive equation V.2, use two facts. First in the thermodynamic limit, we demand that expectations be independent of the order of summing over spins in the configuration sum, provided one remembers that there are conditional probabilities for each spin depending on the rest of the spins. This is one of the DLR (Dobrushin, Lanford, Ruelle) [41] conditions for a state to be an equilibrium state. This tells us that if we get the right probabilities for the values of all the neighbors of a spin (in the sense that if $J_{ij} \neq 0$ then i and j are neighbors), and then use these values to calculate the expectation of a spin, this will be the correct expectation. This says

$$\langle s \rangle^{+} = \langle \tanh(\sum_{j} J_{ij} s_j + h) \rangle^{+}$$

Note that the values of all the external spins enter into the tanh only through their sum. This is a disguised one-variable problem. The second fact we need is that functions that are like tanh satisfy a Jensen - like inequality for certain measures. The important properties of tanh define a class of functions:

Definition: Let M be the class of functions that are odd, positive for positive argument and concave for positive argument.

If the function is f , f is of class M, and the measure $d\rho$, then the Jensen - like inequality is:

$$\int f(x)\, d\rho \leq f\left(\int x\, d\rho\right)$$

Our use will be for $f = \tanh$, $x = s$ and $d\rho$ is the Boltzmann factor for the rest of the spin lattice. The measure $d\rho$ must have the property that it favors positive values of the function x; we will make this more precise later. The proof proceeds by using the DLR equations to reduce the full spin problem to a disguised one variable problem, the FKG inequalities to show that the Boltzmann factor measure is of the desired form, and the Jensen - like inequality to demonstrate the magnetization bound. In all the steps of this proof we use only general inequalities obeyed by all the common one - component spins, hence the proof works for this large class of spins. The function tanh which is particular to spin $1/2$, will be replaced by any function in the class M. The fact that other spin measures give rise to functions in M is the combined result of GKS I, GKS II, and the GHS inequalities.

V.2 A Jensen-like Inequality

We first prove the Jensen - like property. The following theorems and proofs closely follow Slawny [35].

Theorem V.1: If $f \, \varepsilon M$, and the measure $d\rho$ satisfies

$$\rho(x \geq a) \geq \rho(x \leq -a) \tag{V.3}$$

for any positive a, then

$$\int f(x)\, d\rho \leq f\left(\int x \, d\rho\right) \tag{V.4}$$

Proof : We approximate the measure $d\rho$ by a sum of δ - functions. For convenience we let x_i denote the positive values of x with non - zero measure α_i and $-y_j$ denote the negative values of x with non - zero measure β_j. By taking finer and finer grids or better approximations to $d\rho$ we have the result in the limit. We shall take grids that are symmetric around the origin. Let us assume there exists a matrix γ_{ij} that (in effect) interpolates between $\{\alpha_i\}$ and $\{\beta_j\}$ and which has properties to be listed below. Then a proof of the equation V.4 would run:

$$f\left(\sum_i \alpha_i x_i - \sum_j \beta_j y_j\right) = f\left(\sum_i \alpha_i x_i - \sum_{i,j} \gamma_{ij} y_j \frac{x_i}{x_i}\right)$$

(need: $\sum_i \gamma_{ij} = \beta_j$)

$$= f\left(\sum_i \left(\alpha_i - \sum_j \gamma_{ij} \frac{y_j}{x_i}\right) x_i\right) \tag{V.5}$$

(need: $\{y_j > x_i \rightarrow \gamma_{ij} = 0\}$ and $\sum_j \gamma_{ij} \leq \alpha_i$)

$$\geq \sum_i \left(\alpha_i - \sum_j \gamma_{ij} \frac{y_j}{x_i}\right) f(x_i) \tag{V.6}$$

(by concavity)

$$= \sum_i \alpha_i f(x_i) - \sum_{i,j} \gamma_{ij} \frac{y_j}{x_i} f(x_i) \tag{V.7}$$

$$\geq \sum_i \alpha_i f(x_i) - \sum_{i,j} \gamma_{ij} f(y_j) \qquad \text{(V.8)}$$
$$= \sum_i \alpha_i f(x_i) - \sum_j \beta_j f(y_j).$$

Two remarks need to be made. In going from equation V.5 to V.6 we note that the sum of weights $\sum_i (\alpha_i - \sum_j \gamma_{ij} \frac{y_j}{x_i})$ is only less than or equal to one. Even though concavity requires a set of weights whose measure is exactly one, we are all right since we can include the point $x = 0$ for free and give this point the necessary weight for the sum to be one. Second, in the transition between equation V.7 and equation V.8 we use figure 11 to see that

$$y \frac{f(x)}{x} \leq f(y) \quad \text{if} \quad y \leq x$$

for concave functions.

Now we need to show that a matrix γ_{ij} with desired properties exists. We do this by construction. Suppose that there are n α_i's and m β_j's. We start with γ_{nm} and construct the matrix algorithmically.

Step 1 : Set $i = n$ and $j = m$

Step 2 : do while $\{ i > 0 \text{ and } j > 0 \}$

if $\beta_i < (\alpha_j - \sum_{k>i} \gamma_{kj})$ then

$\gamma_{ij} = \beta_i$; for all $a < j$, set $\gamma_{ia} = 0$; $i = i - 1$; go to step 2.

else:

$\gamma_{ij} = \alpha_j - \sum_{k>i} \gamma_{kj}$; $\beta_i = \beta_i - \alpha_j + \sum_{k>i} \gamma_{kj}$; for all $a < i$, set $\gamma_{aj} = 0$; $j = j - 1$; go to step 2.

Step 3 : Stop

See figure 12 . Clearly all elements γ_{ij} are non - negative, $\sum_i \gamma_{ij} = \beta_j$ and $\sum_j \gamma_{ij} \leq \alpha_i$. We remark that the $\leq$ in the last expression is necessary since we know that $\sum_i \alpha_i \geq \sum_j \beta_j$ by hypothesis. If $y_j > x_i$ we know $\gamma_{ij} = 0$ since we are re - parcelling the weights $\{\alpha_i\}$ to cover the weights $\{\beta_j\}$ and by hypothesis one needs at most the measure from x_j outwards to take care of y_j, i.e.,

$$\rho(x \geq y_j) \geq \rho(x \leq -y_j)$$

Thus you don't need to draw on the α_i associated with an $x_i < y_j$ to cover the associated β_j. ∎

V.3 The Slawny Proof

Let us define

$$f_i(x) = \frac{\int s e^{sx} d\mu_i(s)}{\int e^{sx} d\mu_i(s)}$$

which one recognizes as the mean field consistency function for general $d\mu(s)$, and is $\tanh x$ for spin $1/2$. Here x stands for $\sum_i J_{ij} s_j + h$ and s is the spin we are looking at. We now prove Slawny's main result.

Theorem V.2 : The mean field magnetization, defined as the greatest self consistent solution of

$$m = f_i(m \sum_j J_{ij} + h)$$

is an upper bound to the true magnetization.

Proof : The DLR equations [41] tell us that

$$\langle s_i \rangle^+ = \langle f_i(\sum_j J_{ij} s_j + h) \rangle^+ \tag{V.9}$$

If we let $x = \sum_j J_{ij} s_j + h$ then the right hand side of equation V.9 is $\int f_i(x) d\rho$, which is the correct form for Theorem V.1. We can derive some information about $f_i(x)$ for positive x, and by the obvious symmetry $(d\mu_i(s) = d\mu_i(-s))$, related information about negative x. $f_i(x)$ is positive (GKS I), non - decreasing (GKS II), and concave (GHS). Thus $f_i(x)$ is of class M.

We verify that ρ has the correct property as follows. For free boundary conditions,

$$\rho_0(x \geq a) = \rho_0(x \leq -a)$$

By the FKG inequality we know that increasing boundary spins increases the likelihood that spins are up, i.e.,

$$\rho_+(x \geq a) \geq \rho_0(x \geq a)$$

and

$$\rho_0(x \leq -a) \geq \rho_+(x \leq -a)$$

hence

$$\rho_+(x \geq a) \geq \rho_+(x \leq -a).$$

With both f and ρ satisfying the hypothesis of Theorem V.1 we conclude:

$$\begin{aligned} \langle s\rangle^+ &\leq f\,(\langle \sum_j J_{ij} s_j + h\rangle^+) \\ &= f\,(\sum_j J_{ij}\langle s_j\rangle^+ + h) \end{aligned} \tag{V.10}$$

In the thermodynamic limit both $f_i(x)$ and $\langle s_i\rangle^+$ are translation invariant so the i dependence is non - existent. Equation V.10 tells us that $\langle s_i\rangle^+$ lies between 0 and m_{MF} in figure 11, so we conclude

$$\langle s\rangle^+ \leq m_{mean\ field} \quad \blacksquare$$

We emphasize that only the mean field approximation treats the neighbors of a spin only through their summed spin values. It is because we have only one external parameter, i.e., this sum, that we can use Theorem V.1 to get the mean field bound. For the Oguchi approximation the neighbors of the privileged region come into the problem in two parts, the sum of the spin values affecting each member of the privileged region. The analogy to Theorem V.1 would then be a two-variable inequality and correspondingly much harder to deal with.

Chapter VI
Siu: The Oguchi Bound

VI.1 The Oguchi Magnetization Bound

Our original work in the field of magnetization bounds has been to show that the Oguchi magnetization is an upper bound to the true magnetization. For those cases where the three body magnetization is uniquely defined, this too is shown to be an upper bound. The Oguchi and three body methods improve the mean field method by considering a small region in Λ with a certain number of spins and treating the interactions between these spins exactly. These methods work for any region with the right number of spins, even for those regions where the spin-spin couplings J_{ij} are zero. In this case we recover the mean field result and no advantage has been gained. When one chooses a region of spins where the J_{ij} are non-zero, e.g., nearest neighbors, one expects these methods to be improvements on mean field theory. We then say the methods are 'effectively used'. It is believed that the Oguchi magnetization is smaller than the mean field magnetization and the three body magnetization is smaller than the Oguchi magnetization. While we are unable to demonstrate this for all temperatures, we are able to show that the corresponding transition temperatures obey the expected inequalities, i.e.,

$$T_C(true) \leq T_C(symmetric\, 3\text{-}body) \leq T_C(Oguchi) \leq T_C(meanfield)$$

which implies the expected magnetization relations for a region of temperatures. When the approximations are effectively used in a given model, we are able to show that strict inequalities hold for the decreasing sequence of transition temperatures.

We will follow Pearce in reducing the true thermodynamic expectation to a few-variable inequality. We shall be able to demonstrate this resulting inequality for spin $1/2$ by an induction argument. Our basic tool will be the introduction of a dummy spin equation which we couple to our approximating spin equation by means of a ferromagnetic coupling. Ideas along these lines were suggested by Griffiths [42]. After obtaining the magnetization bounds, we derive implicit functions for the magnetizations and implicit functions for the critical temperatures. The monotonicity of the critical temperatures follows from working with the implicit functions. We are able to give alternative derivations of Pearce's Corollary 3 (Theorem IV.2 this thesis) by using these methods and the Griffiths trick [43].

The utility of our method is that it is a reasonably simple procedure and is valid for a large class of models. For spin $1/2$ models these are the strongest results to date for general ferromagnetic coupling. For nearest neighbor models stronger results exist for the magnetization bound (Krinsky [32]) and the transition temperature bound (Krinsky [32], Fisher [30]). Our results are also suggestive of an algorithmic procedure, that of larger and larger regions, that may approach the true magnetization or the true transition temperature for some models. Also suggested is that this procedure may be valid for other spin measures though this remains to be shown.

Following the ideas outlined in chapter IV we rewrite $\Lambda = \bigcup_{\alpha} X_{\alpha}$ where each X_{α} is a copy of some fundamental region X. If there are n sites (and therefore n spins) in X, we denote by $\mathrm{H}_n(X_{\alpha})$ a new m-dependent Hamiltonian constructed in the following manner. Let $\mathrm{H}_n^0(X_{\alpha})$ be the restriction of H to those couplings involving only spins in X_{α}. Then

$$\mathrm{H}_n(X_{\alpha}) = \mathrm{H}_n^0(X_{\alpha}) + \sum_{i \varepsilon X_{\alpha}} J_i(X_{\alpha}) m s_i$$

Examples of $\mathbf{H}_n$ are $\mathbf{H}_2$ and $\mathbf{H}_3$ in chapter II equations II.6 and II.7 respectively. We may view the construction of $\mathbf{H}_n(X_\alpha)$ in terms of selectively breaking bonds in $\mathbf{H}$. When we focus attention to some particular X_α, we isolate this region from the rest of Λ by 'breaking' the bond $J_{ij}s_is_j$ via the substitution:

$$J_{ij}s_is_j = J_{ij}((m-s_i)(m-s_j) + m(s_i + s_j) - m^2)$$

The term $J_{ij}(m-s_i)(m-s_j)$ is part of an exponential that will be replaced by its Taylor series, and so disappears from the Hamiltonian. We are left with terms linear in s_i, i.e., $J_{ij}m(s_i + s_j)$, that are now absorbed into $\mathbf{H}_n(X_\alpha)$.

Theorem VI.1 : If there is an m, m only a function of β, such that

$$\sum_{[s]}\left[e^{-\beta \mathbf{H}_n}\left(\prod_{s_i \varepsilon X}(m-s_i)^{p_i}\right)\right] \geq 0 \tag{VI.1}$$

for all p_i integral and non - negative, then

$$\langle m-s\rangle_{\Lambda,\mathbf{H}} \geq 0$$

<u>Proof</u> : Following Pearce we write

$$\mathbf{H} = \sum_{X_\alpha \subset \Lambda} \mathbf{H}_n(X_\alpha) - \frac{1}{2}\sum{}'(J_{ij}(m-s_i)(m-s_j) - J_{ij}m^2)$$

In the second sum, $\sum'$, we sum over all pairs s_i and s_j, where i and j lie in different X_α's . We have

$$\langle m-s\rangle_{\Lambda,\mathbf{H}} = \mathbf{N}^{-1}\langle (m-s)\exp(\sum{}'\frac{1}{2}J_{ij}(m-s_i)(m-s_j))\rangle_{\Lambda,\sum_\alpha \mathbf{H}_n(X_\alpha)}$$

where

$$\mathbf{N} = \langle \exp(\sum{}'\frac{1}{2}J_{ij}(m-s_i)(m-s_j))\rangle_{\Lambda,\sum_\alpha \mathbf{H}_n(X_\alpha)}$$

We observe that $\mathbf{N}$ is positive. By expanding the exponential in the numerator in a Maclaurin series, the numerator becomes a sum over products, each product factoring over regions X_α. The final expression after factorization is just our hypothesis which is assumed non - negative. By reversing this argument we have the conclusion. The argument concerning the transition to the thermodynamic limit is in chapter II.1. We refer the reader to chapter IV in the proof of Theorem IV.1 to see some of the partial steps written out.

Consider first the Oguchi approximation. Equation VI.1 written out explicitly is

$$\sum_{s,t\,=\,\pm 1} e^{Jst\,+\,k(s\,+\,t)}(m-s)^p(m-t)^q \geq 0 \tag{VI.2}$$

where J is the coupling between spins s and t. As we examine equation VI.2, we observe that some of the difficulty in showing this result comes from the infinitude of possible p and q values. We reduce the number of necessary values to consider by the next lemma.

Lemma : If

$$\sum_{[s]} Ker(m-s)^p s^\alpha \sim (-)^\alpha \quad \text{and} \quad 0 \leq \mathrm{m} \leq 1,$$

then

$$\sum_{[s]} Ker(m-s)^{p\,+\,1} s^\alpha \sim (-)^\alpha$$

The range of values for m is clearly the range of possible expectation values for our spin so this condition is automatically fulfilled. Inspection of equation VI.2 indicates that later useful choices for Ker will be

$$Ker = \exp(Jst + k(s + t))$$

and

$$Ker = \{\exp(Jst + k(s+t))\}(m-t)^q t^b$$

for the Oguchi model. Clearly we can use this induction step in the proof of equation VI.1 for any region X_α.

Proof : Let 'u' be a dummy spin 1/2 variable. For spin 1/2

$$\lim_{K\to\infty} \frac{e^{Ksu}}{\left(\sum_{x,y=\pm1} 2e^{Kxy}\right)} = \delta_{su}$$

so

$$\sum_{[s]} Ker(m-s)^{p+1}s^{a} =$$

$$\lim_{K\to\infty} \frac{1}{\left(\sum_{x,y} 2e^{Kxy}\right)} \sum_{[s],u} e^{Ksu}\, Ker(m-s)^{p}s^{a}(m-u) \tag{VI.3}$$

For any fixed K, using the identity

$$e^{Ksu} = \cosh K + su \sinh K$$

the right-hand side of eq. VI.3 (RHS) is

$$RHS \sim (\cosh K)\Big(\sum_{[s]} Ker(m-s)^{p}s^{a}\Big)\Big(\sum_{u}(m-u)\Big)$$
$$+ (\sinh K)\Big(\sum_{[s]} Ker(m-s)^{p}s^{a+1}\Big)\Big(\sum_{u}(m-u)u\Big)$$

We calculate two of the sums explicitly. In the first sum we may also choose to note that $u(m-u)$ is negative for both values of u so the sign of the sum is seen even without evaluating the sum.

$$\sum_{u}(m-u)u = m\sum_{u} u - 1 = -1 \sim (-).$$
$$\sum_{u}(m-u) = m-\sum_{u} u = m \sim (+).$$

Therefore, using the induction hypothesis, we can write:

$$RHS \sim (+)(-)^{a}(+) + (+)(-)^{a+1}(-).$$

$$\sim (-)^a$$

Since this holds for any K positive, it also holds in the limit and we have

$$\sum_{[s]} Ker(m-s)^{p+1} s^a \sim (-)^a \quad \blacksquare$$

The previous lemma has reduced the proof of the non - negativity of equation VI.1 to a proof of the two statements:

$$\sum e^{Jst + k(s+t)}(m-s)s^a \sim (-)^a \tag{VI.4}$$

and

$$\sum e^{Jst + k(s+t)}(m-s)s^a(m-t)t^b \sim (-)^{a+b} \tag{VI.5}$$

Equation VI.1 is just the case where $\alpha = \beta = 0$ and the above equations imply the necessary non- negativity. We complete the proof of the Oguchi bound in

Theorem VI.2 : Equation VI.1 holds for the Oguchi Hamiltonian.

Proof : Since the spin s is a spin $1/2$ variable, there are really only two values of α to consider, $\alpha = 0$ and $\alpha = 1$. To prove equation VI.4 for $\alpha = 0$, we note that we have not yet specified the value of m. Let us now define $m = m_{Oguchi}$ where m_{Oguchi} is the value of m such that the left-hand side of eq. VI.4 is identically zero for $a = 0$. Explicitly,

$$m = \left(\sum_{[s]} e^{-\beta H_2} s \right) \Big/ \left(\sum_{[s]} e^{-\beta H_2} \right)$$

That takes care of the case a = 0 for eq. VI.4. For a = 1, we notice $s(m-s) \leq 0$ for both $s = \pm 1$ and so the sum must be non-positive. This proves equation VI.4. To see equation VI.5 we rewrite

$$e^{Jst} = \cosh J + st \sinh J$$

and have:

$$\sum e^{-\beta H_2}(m-s)s^a\,(m-t)t^b$$

$$= (\cosh J)(\sum_s e^{ks}(m-s)s^a)(\sum_t e^{kt}(m-t)t^b)$$

$$+ (\sinh J)(\sum_s e^{ks}(m-s)s^{a+1})(\sum_t e^{kt}(m-t)t^{b+1})$$

where H_2 is the Oguchi Hamiltonian (see equation II.5). To determine the sign of $\sum_s e^{ks}(m-s)s^a$, we recall the correlation inequality GKS II. GKS II tells us that a magnetization defined by $H_2 = -Jst - k(s+t)$ is not less than that defined by $H = -ks$. (Intuitively this says that increasing a ferromagnetic coupling can only aid in the alignment of all the spins and thus increase the magnetization, which is reasonable.) Then we know that

$$\sum_s e^{ks}(m-s) \geq 0$$

As before, we know

$$\sum_s e^{ks}(m-s)s \leq 0$$

from the sign of $(m-s)s$. This information about the signs of all the terms tells us

$$\sum e^{-\beta H_2}(m-s)s^a(m-t)t^b \sim (+)(-)^a(-)^b + (+)(-)^{a+1}(-)^{b+1}$$

$$\sim (-)^{a+b}$$

as needed. ■

We remarked before that in all models considered nowadays the expectations of the two spins in the Oguchi approximation are equal. Examination of our proof shows that if one were to construct a model where these expectations were different, the Oguchi approximation would still give an upper bound. This upper bound would correspond to the larger of the two expectations. This argument will not work for the proof of the three body bound given below. Our demonstration of equation VI.7 requires the use of the GKS II correlation inequality, which in turn requires a unique expectation value of the spins.

VI.2 The Three-Body Magnetization Bound

Our first two theorems apply equally well to any region X. To get the three body bound we have:

Theorem VI.3 : (3-body case)

If $X = \{s, t, u\}$ and there is a Hamiltonian H_3 on X such that $\langle s \rangle = \langle t \rangle = \langle u \rangle = m$, then eq. (VI.1) holds.

Proof : The three cases to consider are

$$\sum_{[s]} e^{-\beta H_3}(m - s_i) s_i^a \sim (-)^a \qquad \forall i \,\varepsilon\, X \tag{VI.6}$$

$$\sum_{[s]} e^{-\beta H_3}(m - s_i) s_i^a (m - s_j) s_j^b \sim (-)^{a+b} \qquad \forall i,j \,\varepsilon\, X, i \neq j \tag{VI.7}$$

$$\sum_{[s]} e^{-\beta H_3}(m - s) s^a (m - t) t^b (m - u) u^c \sim (-)^{a+b+c} \tag{VI.8}$$

where again the Lemma brings us to equation VI.1. As before, define $m = m_{3-body}$ where m_{3-body} is the largest m such that the left-hand side of VI.6 is identically zero for a = 0. By the assumed equality of expectation of all three spins s, t, u, this is possible with one value of m. For $a = 1$, we use the non - positivity of $s(m - s)$. This proves case VI.6. Case VI.8 can be shown by rewriting the coupling terms in the Boltzmann factor as cosh and sinh as done in Theorem VI.2. We notice

$$\exp(J_{st} st + J_{tu} tu + J_{su} su) = \prod_{\text{pairs } i,j} (\cosh J_{s_i s_j} + s_i s_j \sinh J_{s_i s_j}).$$

The important point is that the spin variables occur in pairs. In equation VI.8 one sees that changing two (or any even number) of spins at a time doesn't affect the sign of the product

$$(\sum_s e^{k_1 s}(m-s)s^a)(\sum_t e^{k_2 t}(m-t)t^b)(\sum_u e^{k_3 u}(m-u)u^c)$$
$$\sim (-)^{a+b+c}.$$

Thus the left hand side of equation VI.8 will be a sum of three terms, each of which is $\sim (-)^{a+b+c}$ which proves case VI.8. We demonstrate Case VI.7 by using our ferromagnetic coupling trick and by using GKS II which says

$$\langle s\rangle\langle t\rangle - \langle st\rangle \leq 0$$

Let 'y' be a dummy variable. The left-hand side {LHS} of Case VI.7 for $a = 0$ is:

$$\sum_{[s]} e^{-\beta H_3}(m-s)(m-t)t^{b+1} = \lim_{K\to\infty} \sum_{[s],y} \frac{e^{Kty}}{(\sum 2e^{Kxz})} e^{-\beta H_3}(m-s)t(m-y)y^b$$

Fix K. The RHS may be written as:

$$RHS \sim (\cosh K)(\sum_{[s]} e^{-\beta H_3}(m-s)t)(\sum_y (m-y)y^b)$$
$$+ (\sinh K)(\sum_{[s]} e^{-\beta H_3}(m-s))(\sum_y (m-y)y^{b+1})$$

using $s^2 = 1$. We observe that

$$\sum_{[s]} e^{-\beta H_3}(m-t)s \sim \frac{\sum_{[s]} e^{-\beta H_3}(m-t)s}{\sum_{[s]} e^{-\beta H_3}}$$

$$= \langle (m-t)s\rangle_{H_3}.$$

By GKS II this is non - positive. The signs of the above terms are then

$$\sim (+)(-)(-)^b + (+)(+)(-)^{b+1}$$

$$\sim (-)^{b+1}$$

as needed. The case $(a = 1, b = 0)$ may similarly be shown. Since $s(m-s) \le 0$, $s(m-s)t(m-t) \ge 0$ which takes care of the case $a = b = 1$. This exhausts the possibilities and Case VI.7 is shown. ▪

The implicit equations for the three magnetization upper bounds are: (we resurrect the β dependence)

(i) mean field upper bound

$$m = \tanh(\beta(\sum_j J_{ij} m + h))$$

(ii) Oguchi upper bound

$$m = \frac{\sinh(2x\beta)}{\cosh(2x\beta) + \exp(-2\beta J)}$$

(iii) symmetric 3 - body upper bound

$$m = \frac{\sinh 3x\beta + e^{-4\beta J}\sinh x\beta}{\cosh 3x\beta + 3e^{-4\beta J}\cosh x\beta}$$

where x stands for $mJ_i(X) + h$.

VI.3 Proof of the Critical Temperature Bounds

The magnetizations predicted by the Oguchi and three-body Hamiltonians have been shown to be upper bounds on the magnetization of the true Hamiltonian. We expect these magnetization bounds to be a decreasing series as the number of spins in X is increased. To get a quantitative feel for these bounds, we now examine the critical temperatures predicted by these two methods. In this section we will explicitly show the β-dependence.

Theorem IV.4 : Given a Hamiltonian $\mathbf{H}$ we have

$T_c\,(true) \le T_c$ (symmetric three-body) $\le T_c$ (Oguchi) $\le T_c$ (mean field).

We recall that the critical temperature of the approximation schemes are obtained as the solution to

$$\frac{\partial \langle s \rangle_{\Lambda,\mathbf{H}}}{\partial m}\bigg|_{m=0} = 1$$

with the external field $h = 0$. Using the explicit equation obeyed by the magnetization for the mean field approximation, the mean field critical temperature is determined by

$$\beta_{MF} \sum_j J_{ij} = 1. \qquad \text{(VI.9)}$$

The corresponding equation for the Oguchi case is $(\beta_0 \equiv \beta_{Oguchi})$

$$\beta_0 (\sum_j J_{ij} - J)(1 + \tanh J\beta_0) = 1. \qquad \text{(VI.10)}$$

and the symmetric three-body case gives:

$$\beta_3 (\sum_j J_{ij} - 2J)(1 + 2\left(\frac{\tanh J\beta_3 + \tanh^2 J\beta_3}{\tanh^3 J\beta_3 + 1}\right)) = 1.$$

We remark that examination of the proofs below show that equality is obtained only for the pair coupling $J = 0$ and that otherwise one has strictly better bounds.

Proof: Clearly all the critical temperatures are upper bounds to the true transition temperature. We show that

$$\sum_j (\beta_{C,MF} - \beta_{C,Oguchi})\, J_{ij} \le 0$$

which implies that $T_{C,Oguchi} \le T_{C,MF}$. As we are now working only with critical temperatures, henceforth we drop the subscript 'C'. By eqs. VI.9 and VI.10, we have

$$\sum_j J_{ij}(\beta_{MF} - \beta_0) = 1 - \left[\frac{1}{1 + \tanh \beta_0 J} + \beta_0 J\right]$$

Examine the right hand side (RHS). Let $x = \beta_0 J$ and note that x is non-negative. When $x = 0$, the right hand side $=0$. Now

$$\frac{\partial}{\partial x}(RHS) = \frac{1}{(1 + \tanh x)^2} \bullet \frac{1}{\cosh^2 x} - 1.$$

Since this is negative for all positive x, we see that the right hand side is non-positive, as needed.

To show $\beta_3 \geq \beta_0$, we note that if

$$g(x) = (\sum_j J_{ij}\, x \;-\; 2Jx)\left[1 + 2\frac{(\tanh Jx + \tanh^2 Jx)}{\tanh^3 Jx + 1}\right]$$

then $g(x)$ is an increasing function of positive x. We will show that $g(\beta_0) \leq 1$. Since $g(\beta_3) = 1$, this implies that $\beta_3 \geq \beta_0$. If $y = \beta_0 J$ and $T = \tanh y$, clearly

$$y \geq \frac{T}{1+T} \geq \frac{T}{(1+T)} \frac{(1 + T - T^2)}{(1 + T + T^2)}.$$

Then:

$$\frac{1}{1+T} - y \leq \frac{1}{1 + 2\left[\frac{T(T+1)}{T^3 + 1}\right]}$$

But

$$\frac{1}{1+T} - y = \sum_j J_{ij}\beta_0 - 2J\beta_0$$

by equation VI.10 so we've shown $g(\beta_0) \leq 1$.

We present some sample calculational results obtained with these methods. See figure 4. The values for $T_{C,MF}$ and $T_{C,0}$ are obtained from equations VI.9 and

VI.10. We remark that while each of the three spins in the three-body model is predicting zero magnetization, this is a bound on the magnetization. Thus we can obtain an upper bound on T_C, call it $T_{C,3}$, corresponding to $\max_{s \varepsilon X} T_{C,3}(s)$. This is what is listed under T_C 3-body. We emphasize that even though most of the models given below are nearest neighbor, our method is not restricted to nearest neighbor models and gives new and better results to models such as the one-dimensional $1/r^2$ model.

We have numerically plotted the magnetization bounds for various models. They are listed in figure 13 and their generating program in figure 14. Occasional irregularities near the critical point are due to roundoff effects in the computer simulation. As expected, the three magnetization bounds form a decreasing sequence.

VI.4 Rederiving Pearce

Pearce's Corollary 3 (Theorem IV.2 this thesis) may also be demonstrated using the methods of this chapter. We recall this result:

Theorem VI.5

$$\sum_s e^{ks}(m-s)^p \geq 0 \qquad \text{(VI.11)}$$

for spin $1/2$ and spin 1 measures.

Proof : For spin $1/2$ we use the Lemma to reduce the inequality to

$$\sum_s e^{ks}(m-s)s^{\alpha} \sim (-)^{\alpha}$$

For $\alpha = 1$ this is clearly true. As before, for $\alpha = 0$ we use this equation to define m. This gives

$$m = \frac{\sum_s e^{ks} s}{\sum_s e^{ks}}$$

which is the mean field magnetization. This proves the spin $1/2$ case.

For spin 1, we use the Griffiths trick of writing a spin $n/2$ variable as a ferromagnetically pair-coupled system of n spin $1/2$ spins [43]. Our spin 1 variable s can now be written as

$$s = \frac{t+u}{2}$$

with associated probability

$$\frac{1}{3\sqrt{2}} e^{\log\sqrt{2}tu}$$

where t and u are spin $1/2$ variables. For example, when $t = u = 1$, $s = 1$ with probability $\frac{1}{3}$ and when $t = 1$, $u = -1$, $s = 0$ with probability $\frac{1}{6}$. Equation VI.11 now reads

$$\sum_{t,u} \frac{1}{3\sqrt{2}} e^{\log\sqrt{2}tu + (k/2)(t+u)} (m - \frac{t+u}{2})^p \geq 0$$

Using the binomial expansion, this is a sum of terms: $(a + b = p)$

$$\sum_a \frac{1}{2^p} \frac{1}{3\sqrt{2}} e^{\log\sqrt{2}tu + (k/2)(t+u)} (m-t)^a (m-u)^b \geq 0$$

This was proved in Theorem VI.2 to be true if

$$m = \frac{\sum_{t,u} e^{\log\sqrt{2}tu + (k/2)(t+u)} t}{\sum_{t,u} e^{\log\sqrt{2}tu + (k/2)(t+u)}}$$

by symmetry,

$$= \frac{\sum_{t,u} e^{(k/2)(t+u)} \frac{1}{3\sqrt{2}} e^{\log\sqrt{2}tu} (\frac{t+u}{2})}{\sum_{t,u} e^{(k/2)(t+u)} \frac{1}{3\sqrt{2}} e^{\log\sqrt{2}tu}}$$

$$= \frac{\sum_s e^{ks} s}{\sum_s e^{ks}}$$

which is the mean field magnetization. ■

Appendix 1 : The GKS I and GKS II Correlation Inequalities

Let us first state that both of these correlation inequalities hold for more general Hamiltonians than the form given below and that they are valid for other types of functions other than those given below. The version given is sufficient to cover all cases covered in the text. For proofs valid for more general Hamiltonians, as well as analogous proofs of other correlation inequalities, see Sylvester [44].

Theorem A1: [GKS I] For general $d\mu(s)$ satisfying $d\mu(s) = d\mu(-s)$ and a Hamiltonian of the form

$$H = -\frac{1}{2}\sum_{i,j} J_{ij} s_i s_j - \sum_i h_i s_i$$

with ferromagnetic J_{ij} and h_i, we have

$$\langle s_k \rangle \geq 0$$

for any k.

Proof : We use free boundary conditions. We recover this theorem and proof for the case of periodic boundary conditions simply by adding extra ferromagnetic couplings J_{ij}. For plus boundary conditions the theorem follows by increasing the external fields h_i to infinity on the set of sites in $\mathbb{Z}^d \setminus \Lambda$. Recall

$$\langle s_k \rangle = \frac{\int_{[s]} \exp(\frac{1}{2}\beta\sum_{i,j} J_{ij} s_i s_j + \beta\sum_i h_i s_i) s_k}{\int_{[s]} \exp(\frac{1}{2}\beta\sum_{i,j} J_{ij} s_i s_j + \beta\sum_i h_i s_i)}$$

We desire $\langle s_k \rangle \sim (+)$. We can neglect the denominator since it is clearly positive. Expand the Boltzmann factor in the numerator into its Taylor series. Note that every term has a positive coefficient. Now each term is a product over sites, a typical one of which is

$$\int s^n d\mu(s)$$

which is zero for odd n by the plus-minus symmetry of $d\mu(s)$, and positive for even n. Reversing this argument gives the result. ▪

Theorem A2: [GKS II] Under the conditions of Theorem 1,

$$\langle st\rangle - \langle s\rangle\langle t\rangle \geq 0$$

where s, t are any two spins.

Proof : Again we use free boundary conditions. If our Hamiltonian H is a function of $\{s_i\}$, we create a duplicate Hamiltonian $\mathrm{H}^* = \mathrm{H}(\{s_i^*\})$ and note that (we drop the subscript i)

$$\langle f(s)\rangle = \frac{\int_{[s]} e^{-\beta \mathrm{H}(\{s\})} f(s)}{\int_{[s]} e^{-\beta \mathrm{H}(\{s\})}}$$

$$= \frac{\int_{[s],[s^*]} e^{-\beta(\mathrm{H}(\{s\}) + \mathrm{H}^*(\{s^*\}))} f(s)}{\int_{[s],[s^*]} e^{-\beta(\mathrm{H}(\{s\}) + \mathrm{H}^*(\{s^*\}))}}$$

Then we calculate

$$\langle st\rangle_{\mathrm{H}} - \langle s\rangle_{\mathrm{H}}\langle t\rangle_{\mathrm{H}} = \langle s(t - t^*)\rangle_{\mathrm{H}+\mathrm{H}^*}$$

Now we use the 'duplicate variables' trick. If we make the substitution

$$p_i = s_i + s_i^* \qquad q_i = s_i - s_i^*$$

$$s_i = \frac{p_i + q_i}{2} \qquad s_i^* = \frac{p_i - q_i}{2}$$

then

$$\mathrm{H} + \mathrm{H}^* = -\frac{1}{2}\sum_{i,j} J_{ij}(s_i s_j + s_i^* s_j^*) - \sum_i h_i (s_i + s_i^*)$$

$$= -\frac{1}{2}\sum_{i,j} J_{ij}\frac{(p_i p_j + q_i q_j)}{2} - \sum_i h_i p_i$$

and our expectation

$$\langle s_i(s_j - s_j^*)\rangle_{H + H^*} = \langle \frac{(p_i + q_i)}{2} q_j \rangle_{H + H^*}$$

Now look at the sign of $\langle (p_i + q_i) q_j \rangle$ as in the proof of Theorem A1. After expanding and factoring we get a typical term of

$$\int p_i^n q_i^m d\mu(s) d\mu(s^*)$$

with n, m non-negative integral. If m is odd, switching the dummy variables around ($s_i \to s_i^*$ and vice versa) shows that this integral is zero. If m is even and n is odd, the switch ($s_i \to -s_i$, $s_i^* \to -s_i^*$) again shows the integral to be zero. For both m and n even, the integral is positive. ▪

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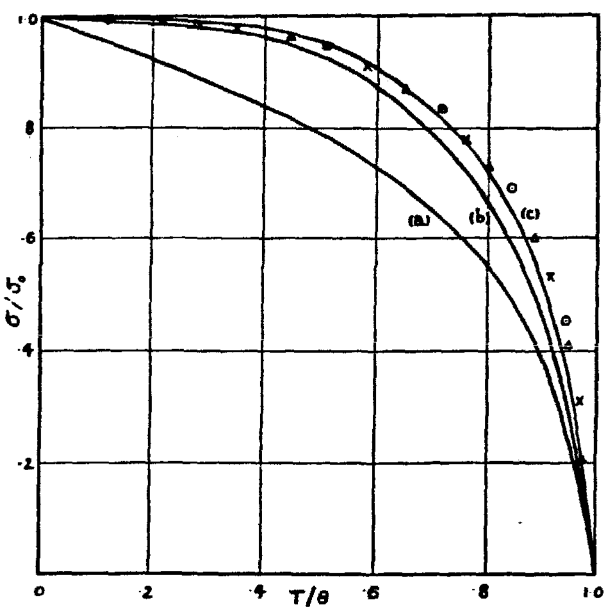

Spontaneous magnetization curves.

(a) Classical curve (Langevin).
(b) Quantum curve, $j=1$.
(c) Quantum curve, $j=\frac{1}{2}$.

⊙⊙⊙, Iron. ××××, Cobalt. △△△, Nickel.

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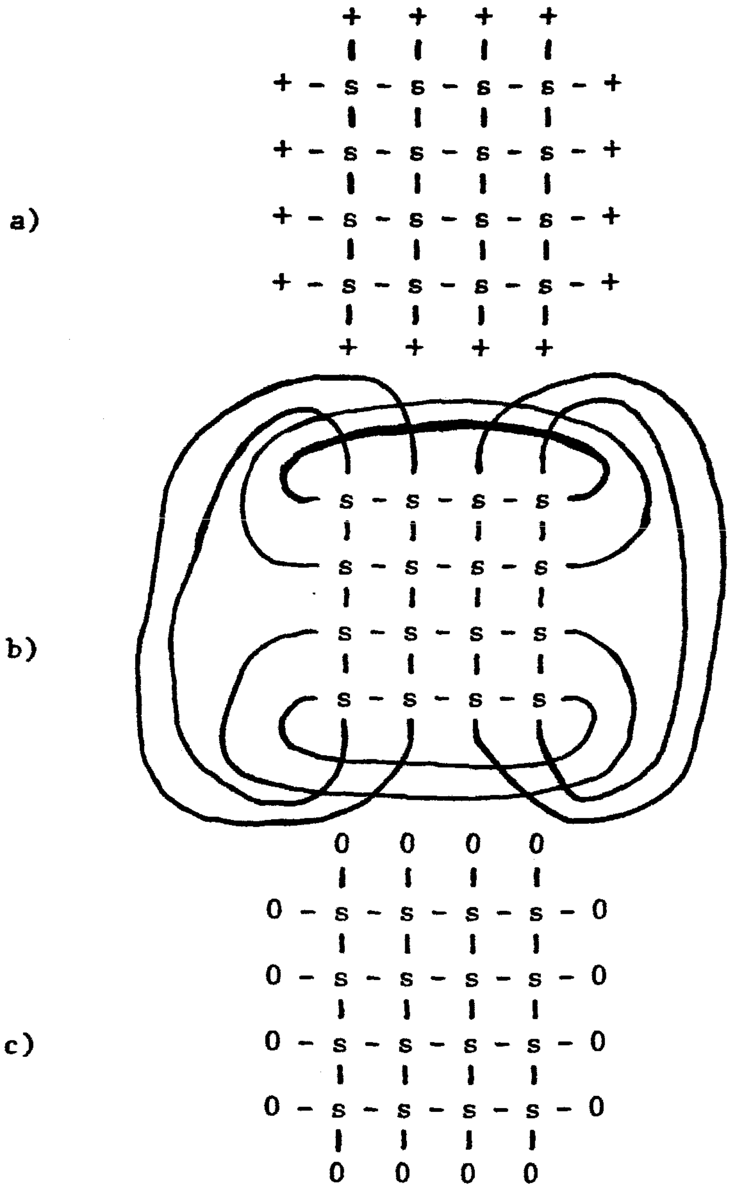
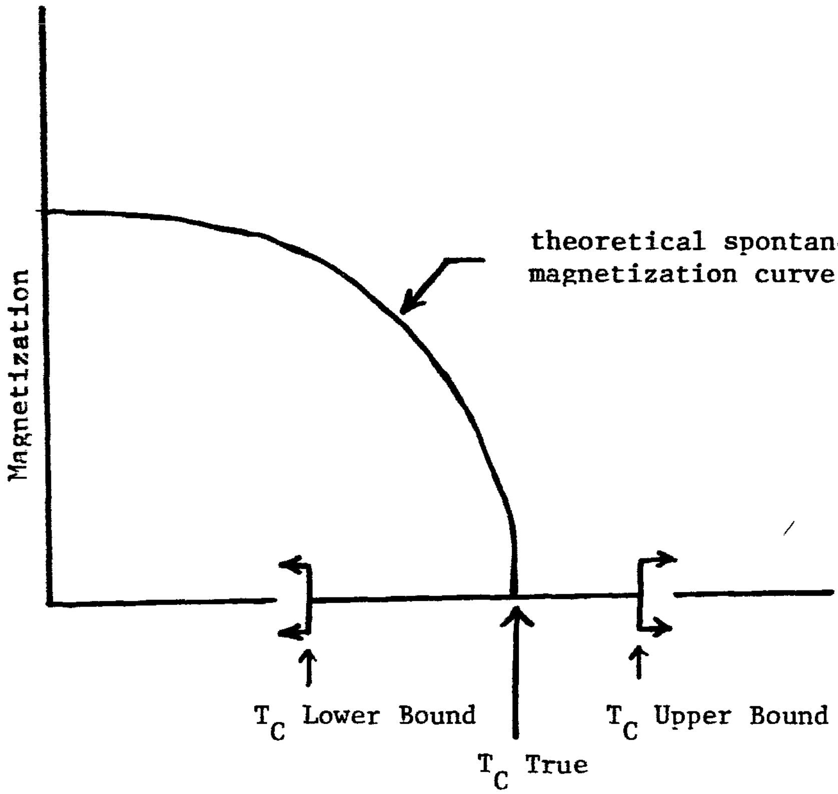
Figure 1



Examples of boundary conditions for a two dimensional nearest neighbor model. 's' stands for a spin. Connecting lines are bonds. a) Plus boundary conditions. b) Periodic boundary conditions. c) Free boundary conditions.

Figure 2



Below T_C Lower Bound the Peierls argument says the magnetization is non-zero. Above T_C Upper Bound Griffiths shows the magnetization is zero.

Figure 3

Critical Temperature Bounds					
Model	Mean Field	Oguchi	3-body	Fisher[a]	Best known
A	4	3.776	3.730	2.885	2.269 *
B	6	5.847	5.825	4.933	4.933[a]
C	3	2.707	2.627	1.820	1.519 *
D	6	5.847	5.641	4.933	3.641 *
E	3.290	3.021	2.897	--	--[b]

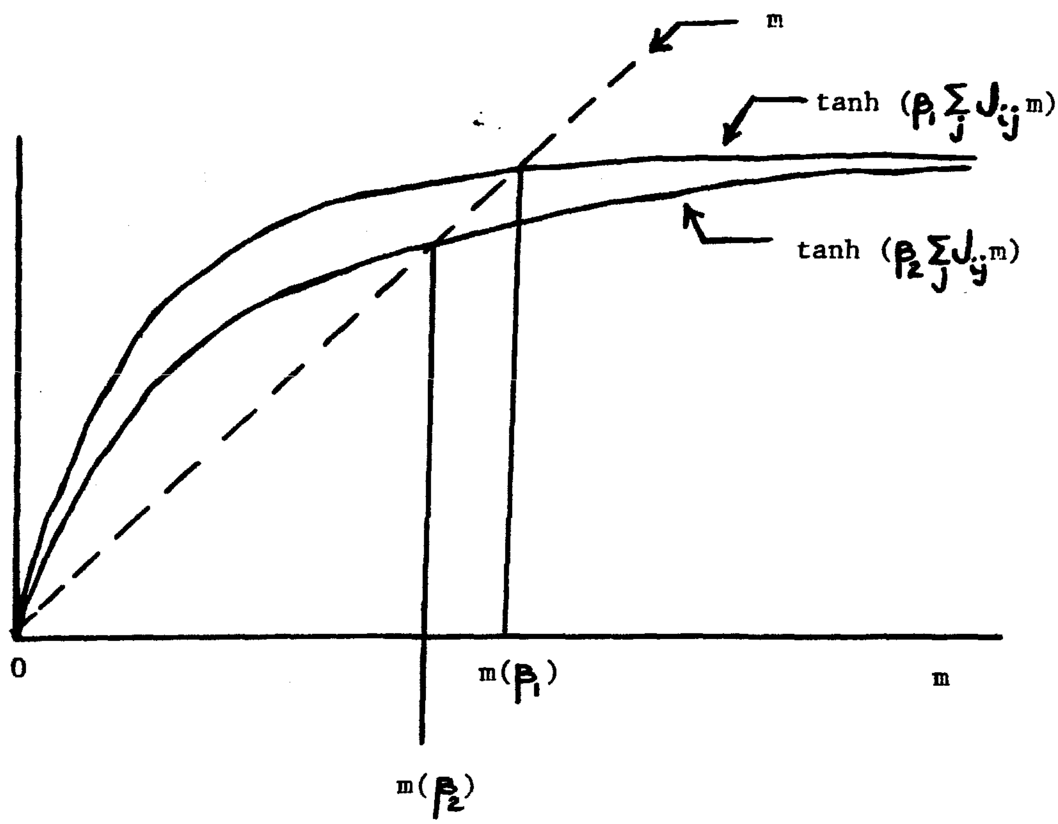
* Exact.

[a] Fisher [30].

[b] Best guess is $T_c \approx 1.58$, Bhattacharjee et. al. [45].

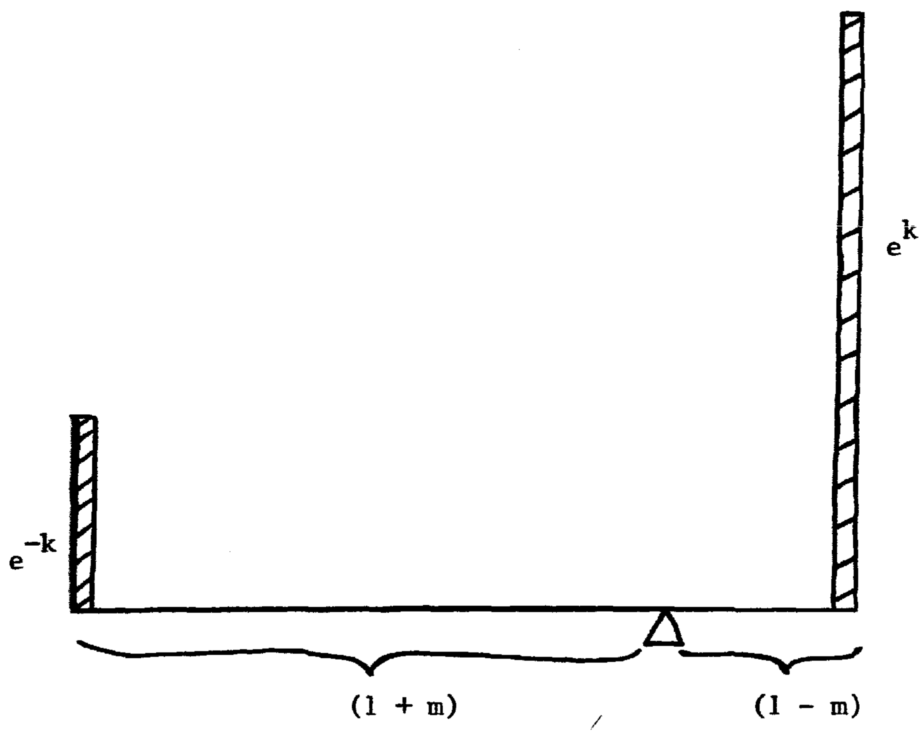
The models are: A = two-dimensional (2-D) nearest neighbor (n.n) square lattice; B = 3-D n.n cubic; C = 2-D n.n hexagonal; D = 2-D n.n triangular; E = 1-D $J_{ij} = |i - j|^{-2}$ model.

Figure 4



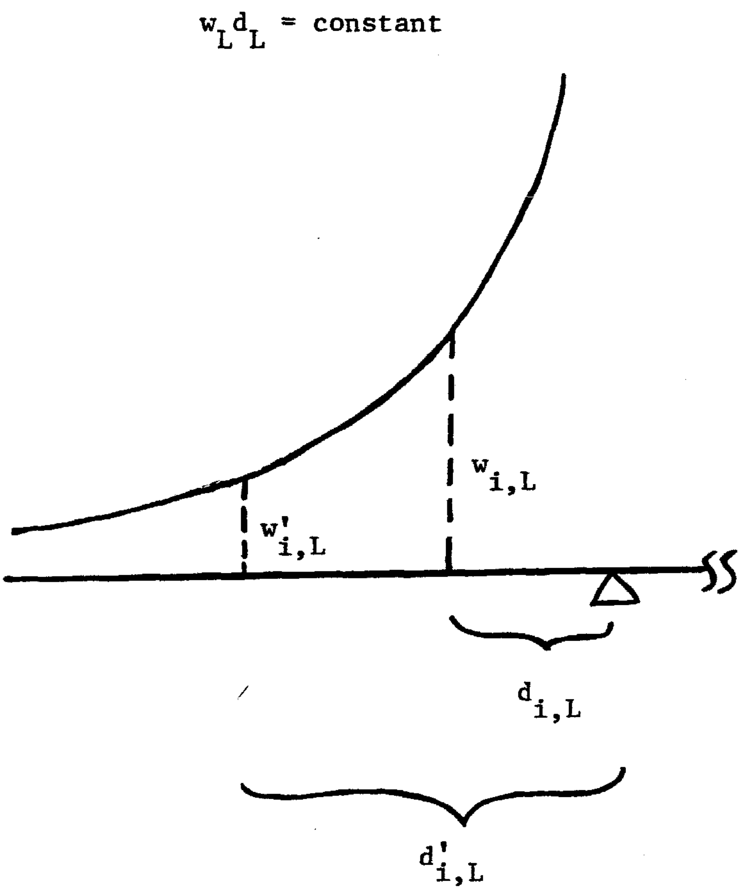
Solving for the mean field magnetization as the intersection of two graphs. Note that the intersection point may be 0 (zero).

Figure 5



A representation of Pearce's inequality as a torque balance problem.

Figure 6



Two pairs of weights and distances contributing the same amount to the determination of the mean. All such pairs lie on the hyperbolic curve shown.

Figure 7

```
      character input,disc_con,nchar
       real    m,k,p,v,sum,mnumer,mdenom,xi,xinc,newval
        integer idummy
      open(unit = 10,file='meanmag.val',status='unknown')
c    +     access='append')
      newval = 0.
      write(6, 5)
      read (5,30)m
      read (5,30)k
      read (5,30)p
      read (5,30)v
      go to 50
2     write(6, 10)
       read (5, 11)input,newval
       if (input.eq.'e')then
          go to 9999
       else if ((input.ne.'m').and.(input.ne.'k')
     + .and.(input.ne.'p')
     + .and.(input.ne.'v'))then
          go to 2
       end if
c  change values of parameters
       if (input.eq.'m') then
         if (newval.lt.0)then
          mnumer = 0.
          mdenom = 0.
          xinc = 2./ v
          xi = -1.- xinc
          do 20 idummy = 1,(v+1)
          xi = xi + xinc
          mnumer = mnumer + exp(k * xi) * xi
20        mdenom = mdenom + exp(k * xi)
          m = mnumer/mdenom
         else
          m = newval
         end if
       else if (input.eq.'k')then
         k = newval
       else if (input.eq.'p')then
         p = newval
       else if (input.eq.'v')then
         v = newval
      end if
```

Standard FORTRAN program written to test Pearce's inequality for arbitrary values of m,k,p and v (for spin v/2). Each time m is set to the correct value, as defined by the p=1 condition, this is indicated with a *. Program ran on a Data General MV4000.

Figure 8

```
50      nchar = '*'
        if (newval.ge.0)nchar = ' '
        call integral(m,k,p,v,sum)
         write(10,90)m,k,p,v,sum,nchar
         write(6, 90)m,k,p,v,sum,nchar
        go to 2
9999    close(unit = 10,status='keep')
        stop
5       format(' initial values of m,k,p,v?
       + (one on a line)(r,r,r,r)')
10      format(' vary? : m,k,p,v,e(xit);
       + value (spon mag: -1.)')
11      format(a1,1x,f8.3)
30      format(f8.3)
90      format(' m: ',f8.3,' k: ',f8.3,' p: ',f8.3,
       + ' v: ',f8.3,' sum: ',f8.3,1x,a1)
        end
c
c
        subroutine integral (m,k,p,v,sum)
        real m, k, v, p, sum, xi, xinc
        integer i, v1, ip
          xinc = 2./v
          v1   = v + 1.
          sum  = 0.
          xi   = -1.- xinc
        do 10 i=1, v1
          xi   = xi + xinc
          if ((m - xi).lt.0.) then
            sum  = sum - (exp(k*xi)) * ((xi - m) ** p)
          else if ((m - xi).ge.0.) then
            sum  = sum + (exp(k*xi)) * ((m - xi) ** p)
          end if
10        continue
        sum = sum / v1
        return
        end
```

Figure 8 (continued)

This program evaluates the sum:

$$\frac{1}{v+1}\sum_{s} e^{ks}(m-s)^{p} \tag{I}$$

(s goes from -1 to 1 in v steps. We divide by $v + 1$ to normalize the measure.)

It allows interactive variation of the parameters:

- m mean field magnetization
- k external field strength
- p real variable
- v 2 * spin of the Ising model

When running the program, a star will be printed at the right when the mean field value of m is computed for a given value of k and v, i.e.,

$$m = \frac{\sum_{v} s e^{ks}}{\sum_{v} e^{ks}}$$

One wants to show that equation I is always positive for:

- k non - negative real
- p non - negative integer
- v all positive integers
- m defined as above

To use the program, input all values as real constants (put in the decimal point) and vary parameters as in this example: m,.67 (The letter of the variable you want changed, followed by a comma and then the appropriate new value. Blank spaces are not recommended.) To exit, type 'e' when asked what to vary. A running log is kept in the file 'meanmag.val' of all parameter values that have been examined.

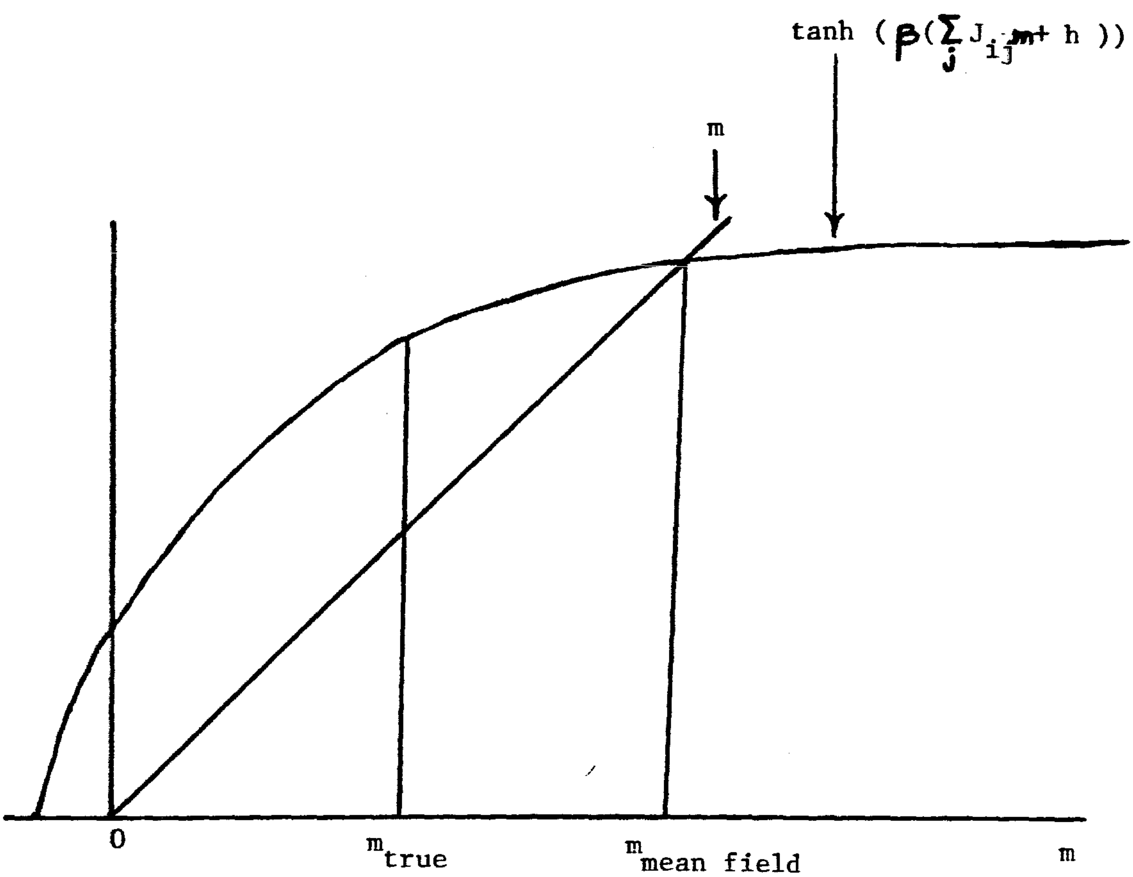
Numerical studies of Pearce's Inequality

m	k	p	v	sum
.055	.1	1.0	3	.000
.055	.1	3.0	3	.042
.055	.1	5.0	3	.090
.055	.1	7.0	3	.145
.269	.5	1.0	3	.000
.269	.5	3.0	3	.196
.269	.5	5.0	3	.431
.269	.5	7.0	3	.766
.496	1.	1.0	3	.000
.496	1.	3.0	3	.324
.496	1.	5.0	3	.736
.496	1.	7.0	3	1.583
.975	5.	1.0	3	.000
.975	5.	2.0	3	.610
.975	5.	2.5	3	.535
.975	5.	3.0	3	.469
.975	5.	4.0	3	.389
.975	5.	5.0	3	.376
.975	5.	7.0	3	.568
.975	5.	9.0	3	.327

Figure 9

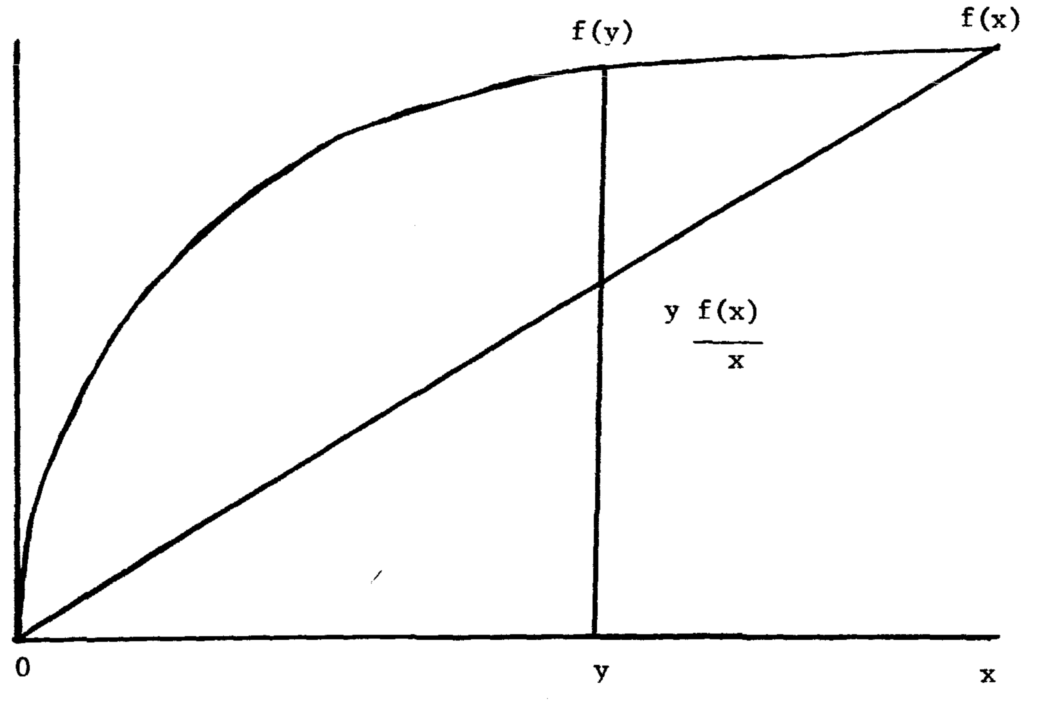
Numerical studies of Pearce's Inequality

m	k	p	v	sum
.050	.1	1.0	4	.000
.050	.1	3.0	4	.032
.050	.1	5.0	4	.066
.050	.1	7.0	4	.102
.243	.5	1.0	4	.000
.243	.5	3.0	4	.153
.243	.5	5.0	4	.314
.243	.5	7.0	4	.530
.453	1.0	1.0	4	.000
.453	1.0	3.0	4	.260
.453	1.0	5.0	4	.549
.453	1.0	7.0	4	1.084
.955	5.0	1.0	4	.000
.955	5.0	3.0	4	.462
.955	5.0	5.0	4	.352
.955	5.0	7.0	4	.529
.997	10.0	1.0	4	.000
.997	10.0	3.0	4	3.838
.997	10.0	5.0	4	1.104
.997	10.0	7.0	4	.440



Graphical illustration of how to recognize when $m_{true} \leq m_{mean\ field}$.

Figure 10



f(x) is a concave function with f(0) = 0.
This is a graphical illustraction that

$$y \frac{f(x)}{x} \leq f(y)$$

Figure 11

$$
\begin{array}{lllll}
\gamma_{11} & \gamma_{12} & \cdots & SS & \\
\gamma_{21} & \cdot\cdot & \cdot\cdot & & \longrightarrow \sum_{k=1}^{m} \gamma_{ik} \leq \alpha_i \\
\cdot\cdot & \cdot\cdot & \cdot\cdot & & \\
\approx & & & & \\
\cdot\cdot & [\beta_{m-2} - \{\alpha_n - \beta_{m-1} - \beta_m\}] & 0 & \cdot\cdot & 0 \\
\cdot\cdot & 0 & [\alpha_n - \beta_{m-1} - \beta_m] & [\gamma_{nm-1} = \beta_{m-1}] & [\gamma_{mn} = \beta_m]
\end{array}
$$

$$\downarrow$$

$$\sum_{k=1}^{n} \gamma_{km-1} = \beta_{m-1}$$

Some steps in the construction of the γ_{ij} matrix. Starting on a given row, one proceeds to fill in the matrix elements going left , stopping when the sum of the entries in that row equals the α associated with that row. The rest of the entries on that row are set equal to zero and one continues to fill in non-zero entries in the matrix element directly above the stopping point. All entries to the right of the new starting point are set equal to zero. One proceeds until one reaches column 1. This matrix is lower triangular.

Figure 12

The following graphs are magnetization graphs calculated from the approximations given on p. 53. The solid line gives the mean field bound, the dotted line gives the Oguchi bound, and the dashed line gives the three-body bound. The three-body bound may or may not be applicable to a given model. This must be checked separately. For the following curves we assumed a nearest neighbor model with the number of nearest neighbors equal to the variable 'Sigma' (corresponding to $\sum_j J_{ij}$), a temperature dependent coupling 'J' (corresponding to βJ), and an external field 'h' (corresponding to h). The program used to draw these plots is listed on p. 85. The parameters used to draw these plots are given below: (T_{max} is only a plotting parameter).

	T_{max}	Sigma	J	h
13a	4	4	1	0
13b	6	6	1	0
13c	12	6	1	1
13d	10	10	1	0

A possible interpretation of these plots consistent with the parameters given is: 13a - two dimensional nearest neighbor (n.n.) model in zero field; 13b - two dimensional triangular or three dimensional n.n. model in zero field; 13c - the models in 13b, but in a non-zero field; 13d - five dimensional n.n. model in zero field. (If not otherwise specified, the underlying lattice is cubic).

Figure 13

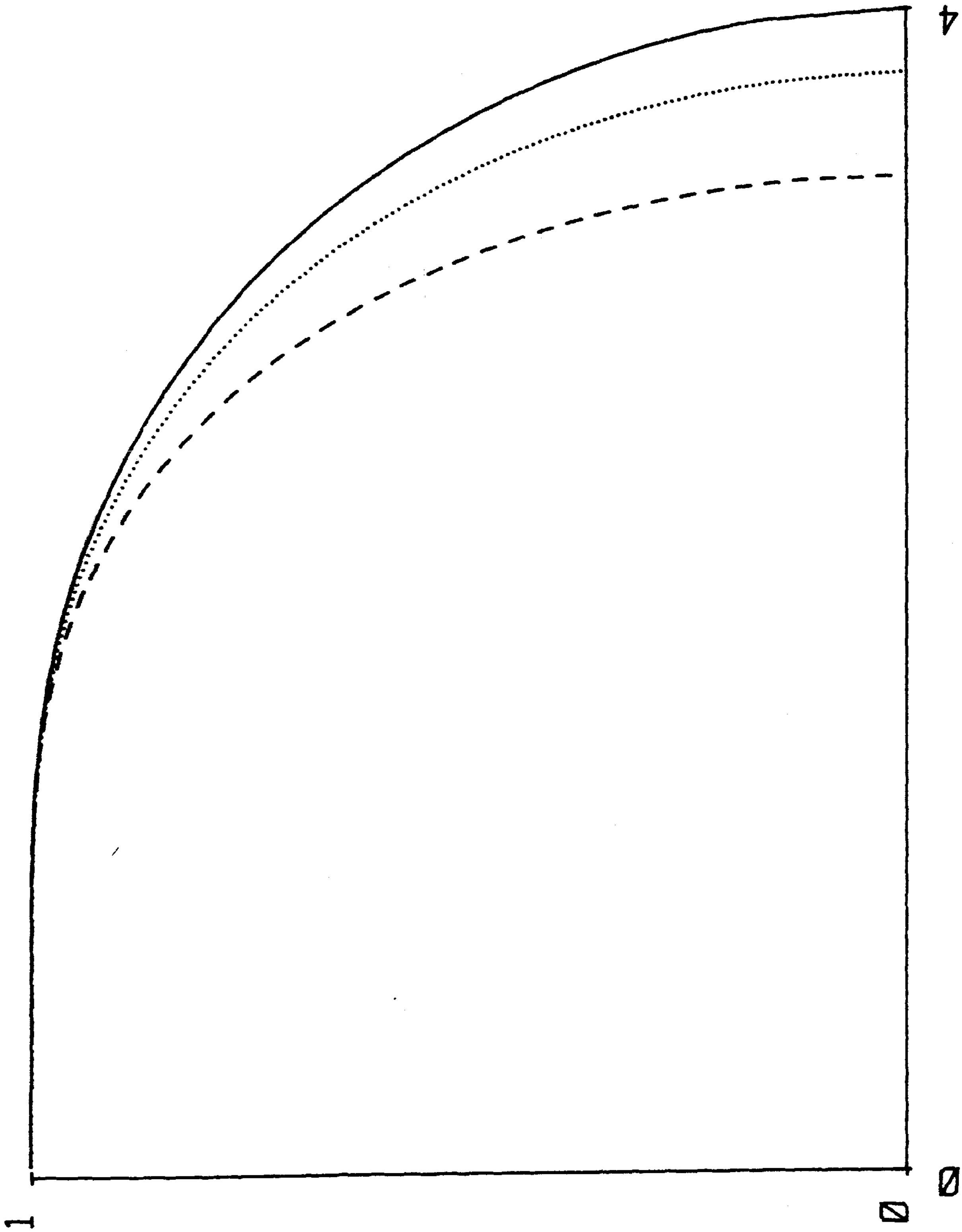


Figure 13a

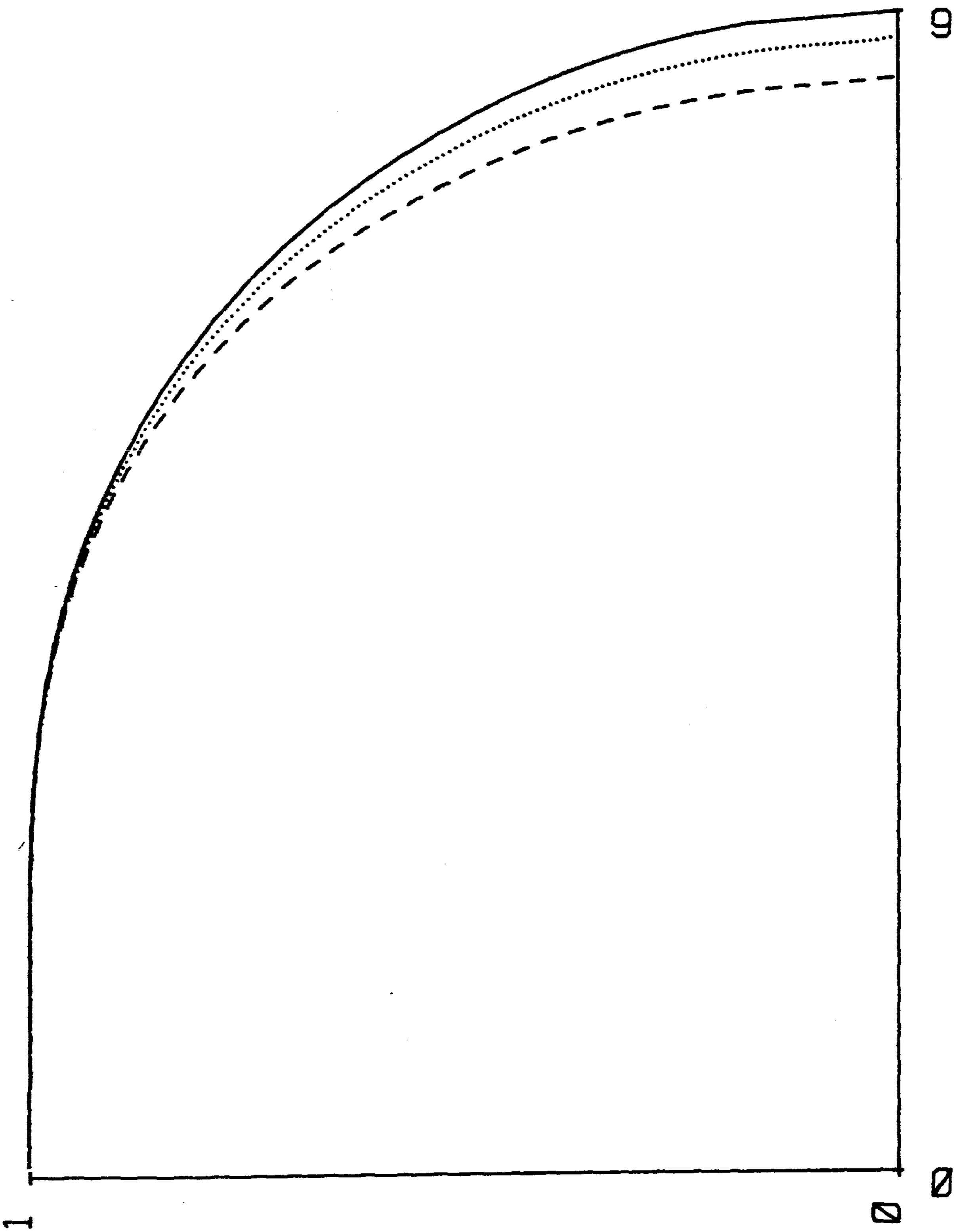


Figure 13b

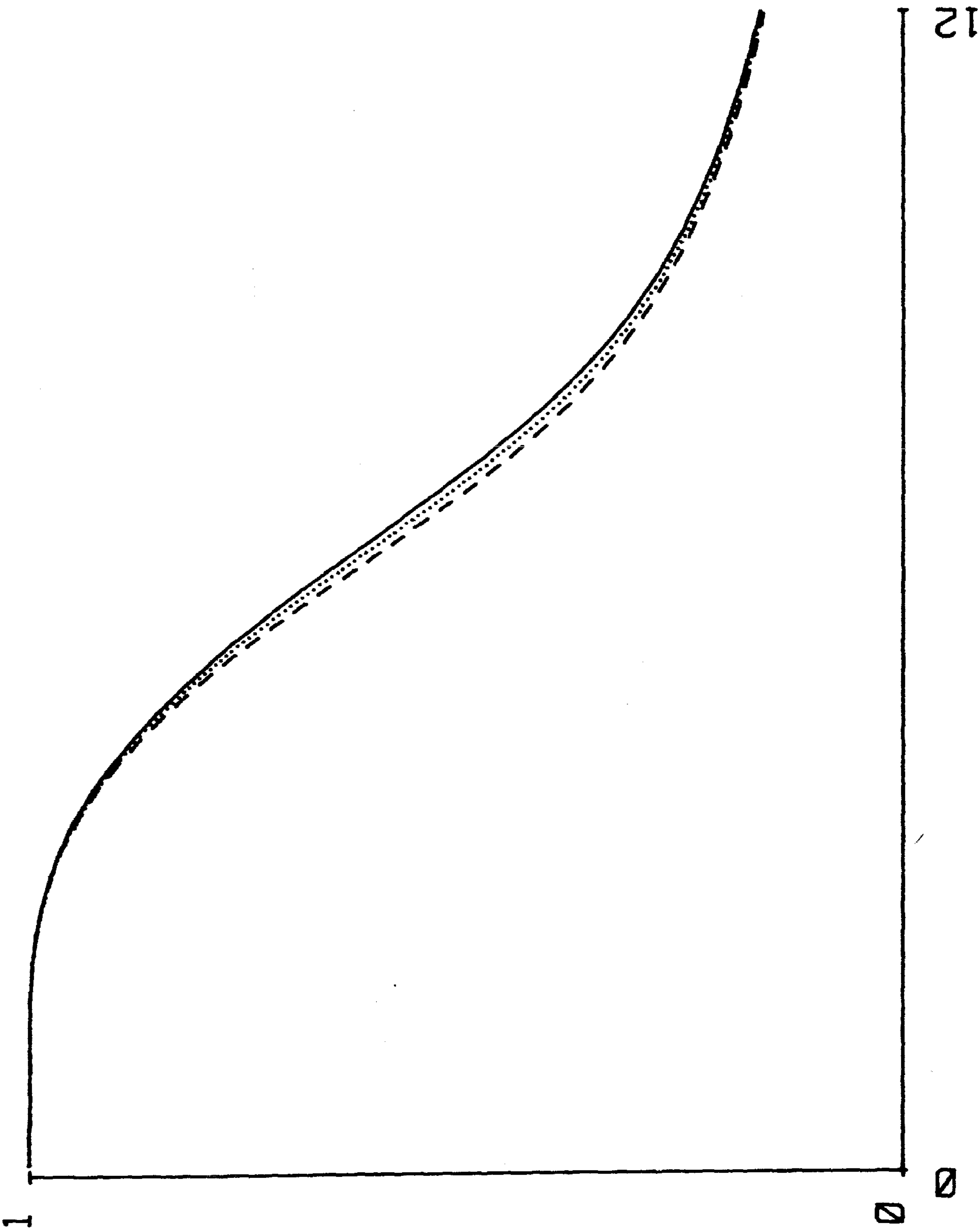


Figure 13c

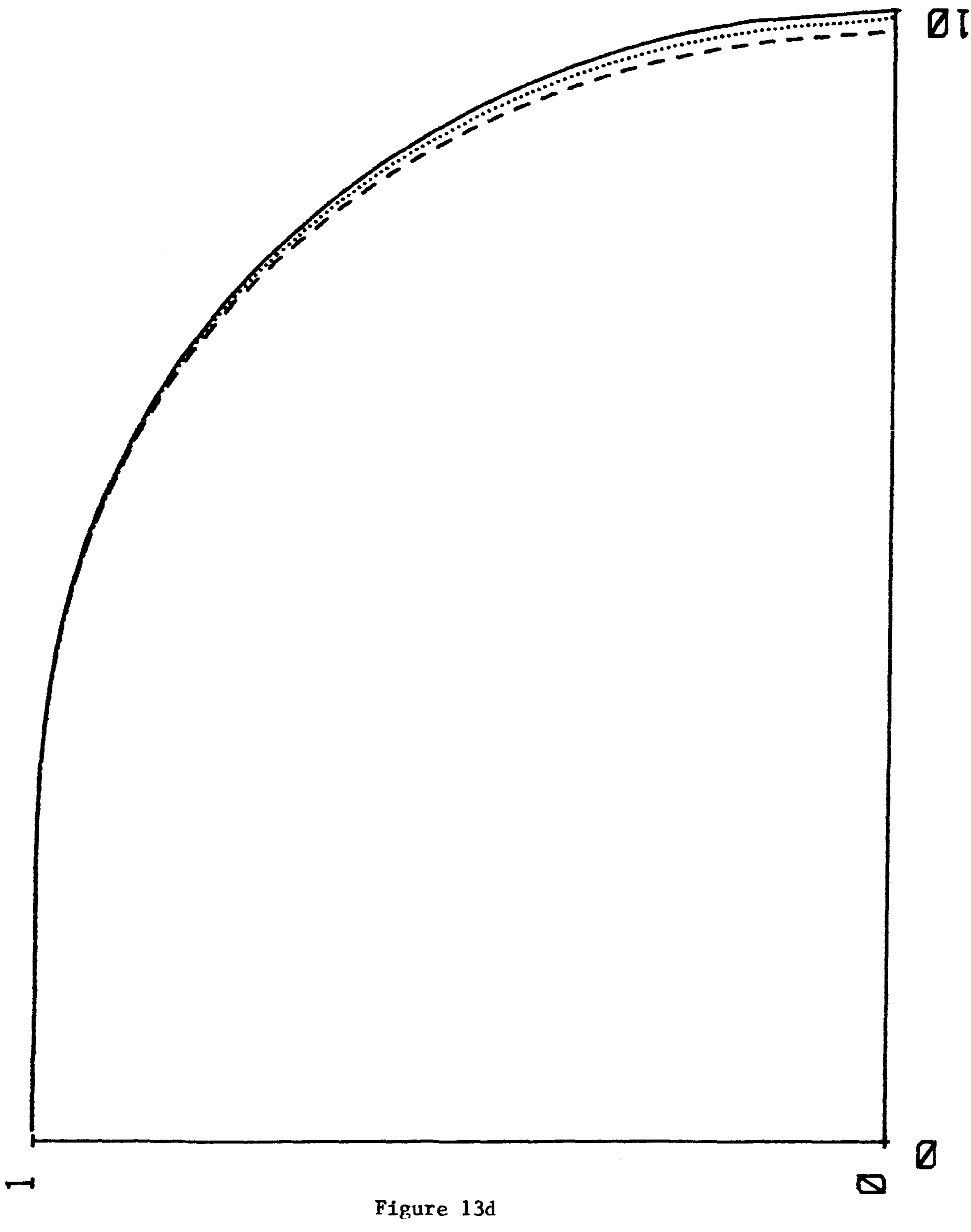


Figure 13d

```
0: "Magnetization Curve Program":
1: pclr;ent "T max ?",U;ent "Sigma ?",S;ent J,H;csiz 3
2: wrt 705,"IP1200,1000,8700,6700";wrt 705,"VS6";line
3: fxd 0;pen# 1;scl 0,U,0,1;xax 0,U,0,U,1;yax 0,1,0,1,1
4: 1→M;for T=U/100 to U by U/100;1/T→B;.01→N;M+N→M
5: M-N→M;if 'f1'(M)<0;gto +0
6: M+N→M;N/10→N;gto -1;if N=1e-4;gto +1
7: plt T,M,1+(T#U/100);if M<=1e-3;pen;gto +2
8: next T;pen
9: line 1,.5;1→M;for T=U/100 to U by U/250;1/T→B;.01→N;M+N→M
10: M-N→M;if 'f2'(M)<0;gto +0
11: M+N→M;N/10→N;gto -1;if N=1e-4;gto +1
12: plt T,M,1+(T#U/100);if M<=1e-3;pen;gto +2
13: next T;pen
14: line 2,2;1→M;for T=.5 to U by U/250;1/T→B;.01→N;M+N→M
15: M-N→M;if 'f3'(M)<0;gto +0
16: M+N→M;N/10→N;gto -1;if N=1e-4;gto +1
17: plt T,M,1+(T#.5);if M<=1e-3;pen;stp
18: next T;pen;stp
19: "f1":ret 'th'(B(Sp1+H))-p1
20: "f2":H+(S-J)p1→p2;ret 'sh'(2Bp2)/('ch'(2Bp2)+exp(-2JB))-p1
21: "f3":H+(S-2J)p1→p2;'sh'(3Bp2)+exp(-4BJ)'sh'(Bp2)→p3
22: ret p3/('ch'(3Bp2)+3exp(-4BJ)'ch'(Bp2))-p1
23: "sh":ret (exp(p1)-exp(-p1))/2
24: "ch":ret (exp(p1)+exp(-p1))/2
25: "th":ret 'sh'(p1)/'ch'(p1)
```

Program to plot magnetization curves for the mean field, Oguchi and three-body methods. Program ran on an HP desktop computer 9825B attached to an HP plotter 9872A.

Figure 14