Studies on the Linear Ising Model and Related Systems

A thesis submitted by Klaus K a n n e m a n n

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Mich jedenfalls blickt da manches an, zum Beispiel:
Minus mal minus is plus – wieso ist minus mal minus
gleich plus, was heißt das, wer ist darauf gekommen,
wem stieg dieser Irrsinn plötzlich in die Nase,
das ist keine Logik und Psychologie, keine Kausalität
und keine Errechnung, das ist zwar ein unlöslicher
Bestandteil der Mathematik, aber doch reine Phantasmagorie,
jenseitiges Spiel und nur als isolierter Ausdruck
seiner selbst zu fassen.

DER PTOLEMÄER

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And thirdly,I wish to convey my gratitude for the additional financial support received from T H E P R O V I N C E O F O N T A R I O during this final year.

August 197o

K. Kannemann

Abstract

The linear Ising model and the associated linear lattice fluid are studied in this thesis.Closed form solutions of the partition functions for models having finite range interaction potentials are obtained and compared with solutions for models having modified long range interaction potentials.The existence of a change of phase is explicitly demonstrated for the latter models whereas,in contrast, the models having first and second order interaction potential are shown to undergo no change of phase.

A mathematical "mechanism" is discovered which describes the spontaneous magnetisation of the linear Ising model having modified long range potential and an analogous result is obtained for the linear lattice fluid with modified long range interaction potential between the component systems.

Finally,an operator formulation is explicitly constructed for the linear models with arbitrary order of interactions : this operator principle is easily extended to models of higher dimension, again with arbitrary order of interactions.The thesis makes use of some concepts of set-theory and employs a result from the theory of measure and integration.

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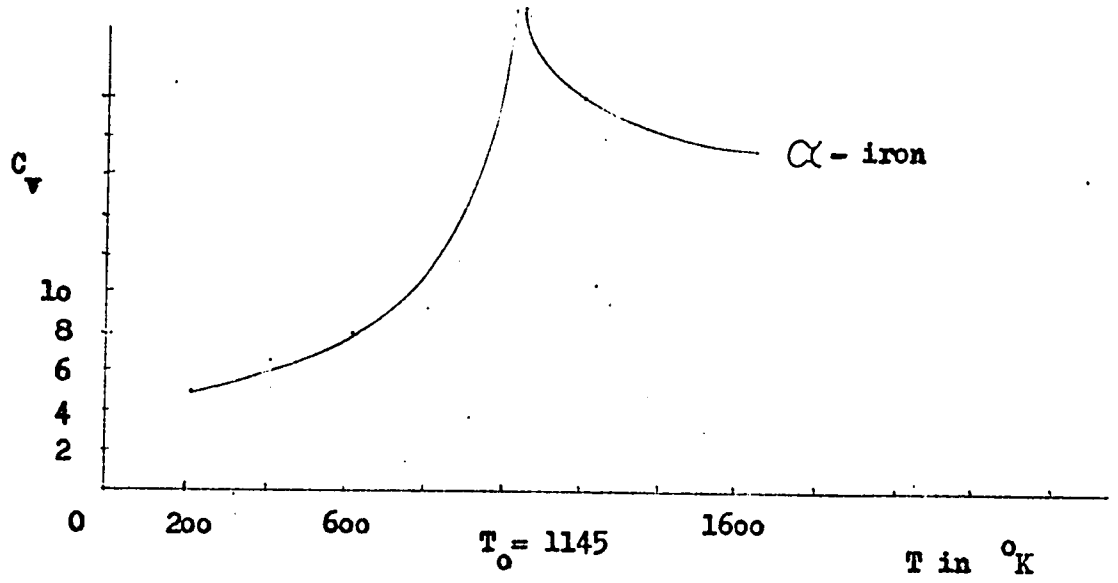
Introduction

§ 1 The context of the problem and a brief historical note.

While an explicit description of the Ising model (and its related lattice fluid) is deferred until chapter II , we find it nonetheless appropriate to give a brief outline of the context in which the problem occurs.

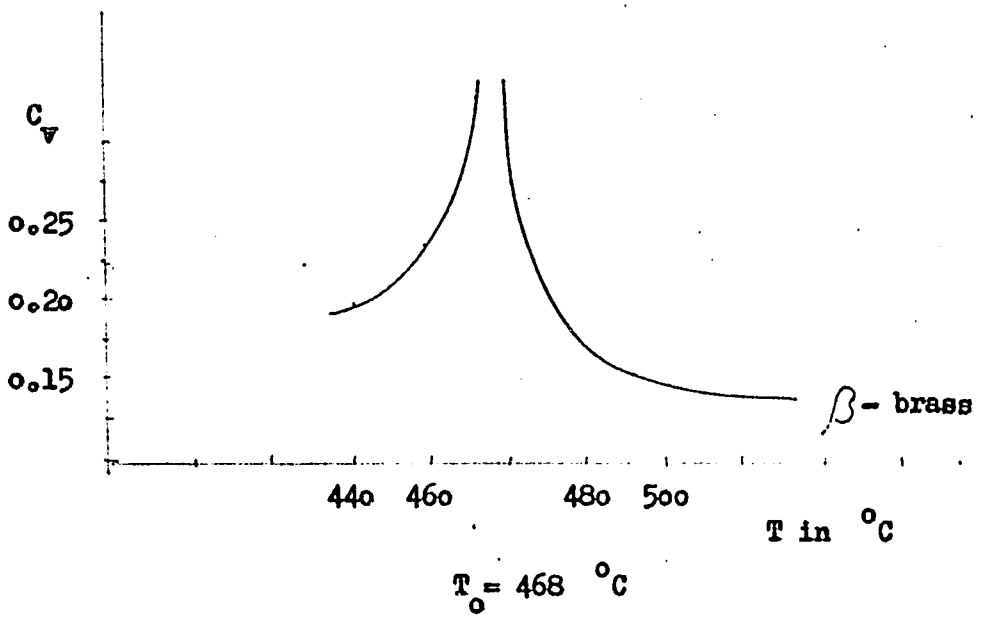
One of the most interesting phenomena of solid state physics is ferromagnetism.It is experimentally established that if a natural magnet is heated above a certain critical temperature,then its natural magnetic field ceases to exist as soon as the critical temperature is exceeded. The same process is observed,experimentally,in reverse order.For example, the below-shown graph,giving a specific heat versus temperature plot for α- iron,was experimentally established.The peak in the curve for α- iron occurs at the temperature at which ferromagnetism disappears.



(The graph is taken from SEITZ: PHYSICS OF METALS , McGraw - Hill)

Equally fascinating are the phenomena of phase changes.Here,most frequently discussed are : condensation,solidification of matter in general,as well as changes in the ordered structure of crystalline substances.The complete collapse of the order structure is identified with melting.

Below, we give a typical graph of the specific heat versus temperature for β - brass (50,4 % Zn) in the critical temperature range where order disappears (after DARKEN and GURRY : Physical Chemistry of Metals).



All such data was obtained by performing macroscopic experiments, that is performing measurements on a sufficiently large piece of matter which, necessarily contains an extremely large number of constituent component systems (molecules, atoms etc.). Our work, then, is devoted to the mathematical description of such and similar phenomena and, in spirit complementary to empirical data stemming from experiments, our data is <u>derived</u> from first principles by investigating the mathematical properties of a suitably chosen m o d e l .

Almost being a misnomer, the "Ising model" was first proposed by W.LENZ in 1920. E.ISING , then a graduate student working with Lenz , investigated the ferromagnetic properties of the one-dimensional (straight line version) model of an assembly of micromagnets (spins) and he succeeded in showing that this model cannot exhibit ferromagnetism , if the mutual interactions between the spins is restricted to nearest neighbours only. His mathematical approach was a combinatorial one. Ising erroneously concluded that the two-dimensional lattice, having nearest neighbour interactions only, cannot exhibit spontaneous magnetisation.

E.MONTROLL reformulated in 1941 the problem for the two-dimensional model by expressing its partition function in terms of the eigenvalues of a matrix.Subsequently, L.ONSAGER obtained in 1944 the exact solution for the partition function and showed that the model undergoes a change of phase which is indicative for spontaneous magnetisation.Onsager 's result has subsequently been rederived by a number of authors,most notably is the solution by spinor analysis given in the paper by B.KAUFMANN and splendidly demonstrated in the fine textbook of K.HUANG : STATISTICAL MECHANICS , (I).

The reader,interested in a more detailed outline of the history of the Ising model,is referred to the exposition by S.G.BRUSH : HISTORY OF THE ISING MODEL , UCRL publication No 794o.This paper also provides an exhaustive reference list of publications on the Ising model.

§ 2 The mathematical apparatus of statistical mechanics. Ensembles.

The notion of an ENSEMBLE is due to GIBBS. Given a macroscopic ASSEMBLY of a very large number of COMPONENT SYSTEMS , we define a MACROSTATE of this assembly as a condition described by the THERMODYNAMIC STATE FUNCTIONS of the assembly, that is : P (pressure) , V (volume) , the temperature T and the molar composition in terms of the molar fractions $n_1, n_2, \ldots$, of the different types of component systems making up the assembly. The state functions P, V and T can be determined by independent experimental arrangements to a sufficient degree of accuracy and the molar composition is subject to chemical analysis. An assembly is said to be in THERMODYNAMIC EQUILIBRIUM if the macrostate is virtually constant in time. An assembly in thermodynamic equilibrium is furthermore described by the EQUATION OF STATE which is a functional relation of the form $f(P,V,T,n_1,n_2, \ldots) = 0$.

When applicable, the equation of state leaves only two state functions independent and we have relations of the form $P = P(V,T)$, $V = V(P,T)$. The internal energy U of the assembly is a function of the state and is independent of the path along which the assembly is displaced from one equilibrium state to another ; the negation of this implies the existence of an inexhaustible source, or insatiable sink of energy.

Given that a macrostate is determined, there exist in general a vast collection of MICROSTATES which are compatible with this macrostate in the sense that if the assembly moves through this set of microstates, the macrostate remains unchanged. The microstate is defined as the instantaneous internal arrangement of the component systems.

If each component system of the assembly has n degrees of freedom, then the entire assembly has Nn degrees of freedom, N being the number of component systems. For assemblies described as macroscopic, N is generally an extremely large number.

Set Nn = S and then we have S generalised coordinates and S generalised conjugate momenta,usually denoted by q_i and p_i ,respectively.A microstate is completely determined by a 2S-dimensional vector:

$$(q_1, \ldots, q_s, p_1, \ldots, p_s) = (q,p)$$

which is also called a point in PHASE SPACE and we write accordingly:

$$(q,p) \in \Gamma = \prod_{i=1}^{s} R_i \otimes \prod_{i=1}^{s} K_i$$

where $q_i \in R_i$ and $p_i \in K_i$. The phase space Γ is therefore the direct product of the CONFIGURATION SPACE and the MOMENTUM SPACE each of which is a product space by itself.

Thus to a determined macrostate there corresponds a point set W in Γ such that the assembly can move through W without affecting its macrostate.The set W represents the DEGENERACY of that macrostate.

GIBBS reinterpreted this notion.Instead of considering the points of W as microstates available to but one assembly and attained by some chance mechanism,he imagined a large number of identical editions of one assembly each brought into correspondence with a point in W.If to each point in W corresponds at <u>least one assembly</u> then this set of assemblies is called an ENSEMBLE.The members of the ensemble are therefore identical assemblies but each being in a certain microstate (but all correspond to the same macrostate) and there can be many in the same microstate.Consequently, the number of member assemblies sharing the same microstate can be considered as a measure of the relative probability that the <u>one assembly</u> under physical consideration be found in that microstate.If this probability is defined and normalised,we have a probability measure on W,or if W is a discrete set we have a probability.

Accordingly, we must have: $\int_W dP(q,p) = 1$, or $\sum_W P(q,p) = 1$

It is now meaningful to speak of the PHASE AVERAGE of a physical observable $O(q,p)$:

$$\langle O \rangle = \int_W O(q,p)\,dP(q,p) \quad , \text{ or } \quad \langle O \rangle = \sum_W O(q,p)P(q,p)$$

Thus phase average is just another word for mathematical expectation. Of course if O is that observable which determines the ensemble:

$$W = \{ (q,p) \in \Gamma \ , \quad O(q,p) = \text{constant} \}$$

then $\langle O \rangle = O(q,p)$ on all of W. We proceed to discuss the three ensembles most frequently applied and relevant to the main part of our work.

<u>The constant energy ensemble - the microcanonical ensemble:</u>

Let $E(q,p)$ be the internal energy of the assembly at (q,p) and consider the set:

$$W = \{ (q,p) \in \Gamma \ , \quad E(q,p) = E_o \ , \text{ constant} \}$$

The set W defines the microcanonical ensemble. The point set W can be considered as the constant energy surface in Γ and more briefly denoted by $W(E_o)$. The probability measure is:

$$dP(q,p) = \frac{dS}{\text{mes}W(E_o)\ \text{grad}\ E}$$

where:

$$\text{mes}W(E_o) = \int_{W(E_o)} \frac{dS}{\text{grad}\ E} \quad , \ dS = : \text{surface element on } W(E_o)$$

The quantity $\mathrm{mes}W(E_o)$ is called the microcanonical PARTITION FUNCTION and it is related to the thermodynamic entropy by the formula:

$$S(E,V) = k \ln \mathrm{mes}W(E)$$

Other thermodynamic functions as well as the equation of state can be derived from $S(E,V)$. The microcanonical ensemble is rarely applied to a discrete phase space.

The constant temperature ensemble - the canonical ensemble.

The probability is defined on the entire phase space Γ. If the phase space is discrete and at most enumerable, we assign to each microstate an integer $i = 1,2, \ldots$ The probability that an assembly of N component systems be found in a microstate i having internal energy $E(i)$ is given by:

$$P(i) = P(E(i)) = \frac{\exp(-\beta E(i))}{Z_N} \quad , \quad \beta = \frac{1}{k\,T}$$

and $Z_N = \sum_i \exp(-\beta E(i))$ is called the canonical partition function.

The energy spectrum is discrete and can have degeneracies. The 2S generalised variables may vary continuously and then we have a probability density:

$$\rho(q,p) = A \exp(-\beta H(q,p))$$

where $H(q,p)$ is the Hamiltonian of the assembly. The canonical partition function is now given by:

$$Z_N = A^{-1} = \int_\Gamma \exp(-\beta H(q,p))\, d\Gamma$$

where $d\Gamma = C\, dqdp$ and C is a constant suitably chosen so as to remove the physical dimension of distance x momentum from Z_N.

The partition function Z_N is related to the HELMHOLTZ free energy F of thermodynamics by the formula:

$$-\beta F(V,T) = \ln Z_N$$

All the other thermodynamic functions as well as the equation of state can be derived from this relation.

The grand canonical ensemble:

We recall that up to now ensemble meant a collection of identical assemblies in different microstates all of which are compatible with a specified macrostate. This is extended now so as to include all the assemblies which can be derived from the one under physical consideration by making the number of component systems a (discrete) variable.

The probability that the assembly be in a state i with energy E(i) and having N component systems is:

$$P(i,N) = P(E(i),N) = \frac{\exp(-\beta(E(i) - N\mu))}{N! \quad \mathcal{Z}}$$

where μ = chemical potential per component system. The factorial is to reduce the degeneracy due to the permutation of N identical but in principle distinguishable component systems. Such a permutation would not create a new physical state. The reduction of this degeneracy is said to result in the proper BOLTZMANN COUNT. The quantity $\mathcal{Z}$ is called the grand canonical partition function and it can be written as the sum:

$$\mathcal{Z} = \sum_{N=0}^{\infty} \frac{\exp(\beta N\mu)\ Z_N(V,T)}{N!}$$

The grand canonical partition function is related to the equation of state by the formula:

$$\frac{PV}{kT} = \ln \mathcal{Z}$$

All other thermodynamic functions as well as the particle density expectation value can be derived from this relation.

Let us briefly return to the HELMHOLTZ free energy F as given in terms of the canonical partition function for an assembly having N component systems:

$$F = - k T \ln Z_N$$

On the other hand, classical thermodynamics defines F in terms of the internal energy U and the entropy S by:

$$F = U - TS$$

It is meaningful to consider the free energy per component system:

$$f_N = \frac{F}{N} = \frac{U}{N} - T \frac{S}{N} = u_N - T s_N$$

so that: $$f_N = - \frac{k T}{N} \ln Z_N$$

The division is well defined indeed, for the temperature T is an intensive property of matter, whereas u_N and s_N are the internal energy, and entropy per component system, respectively.

A macroscopic assembly has generally an extremely large number of component systems (a molar volume at STP has $6{,}023 \cdot 10^{23}$ molecules) and we indicate this by taking the limit:

$$f = \lim_{N \to \infty} f_N = - k T \lim_{N \to \infty} \frac{1}{N} \ln Z_N$$

so that f is the free energy per component system of a macroscopic assembly. We define in the same spirit the specific volume v per component system in terms of the grand canonical partition function:

$$\frac{Pv}{kT} = \lim_{N \to \infty} \frac{PV}{NkT} = \lim_{N \to \infty} \frac{1}{N} \ln \Xi$$

The ISING model and related systems. Description of the models.

§ 1) The ISING model

The Ising model p e r s e is a model for the statistical theory of ferromagnetism. The collective behaviour of particle spin is under investigation here. The magnetic moment associated with particle spin may assume only two coaxial orientations which are usually denoted by spin up, (+), and spin down, (-). This of course corresponds to spin 1/2 in quantum mechanics. If, in the absence of an external magnetic field and below a temperature T_c, the majority of spins tend to align parallel with only comparatively few deviating from this tendency, then we speak of spontaneous magnetisation and the temperature T_c is called the CURIE POINT.

The Ising model consists of a lattice whose sites are occupied by particles with spin described as above. The three basic lattices are:

i) one dimensional : straight line version

ii) two dimensional : plane square version

iii) three dimensional : solid cube version

There are certain advantageous modifications which we describe as identifications:

ia) 1-dim. model : identify N+1st site with the 1st one and obtain the ring model,

iia) 2-dim. model : identify N+1st row with the 1st one and N+1st column with the 1st column and obtain the torus model. If only one identification is carried out one obtains the cylinder model.

Analogous identifications can be done on the three dimensional model. These identifications simplify the mathematical approach considerably. Models with these identifications are said to have PERIODIC BOUNDARY CONDITIONS.

Shown below are the schematics for the ring and the torus model:

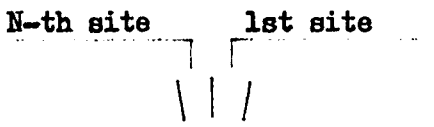


Fig. 1a

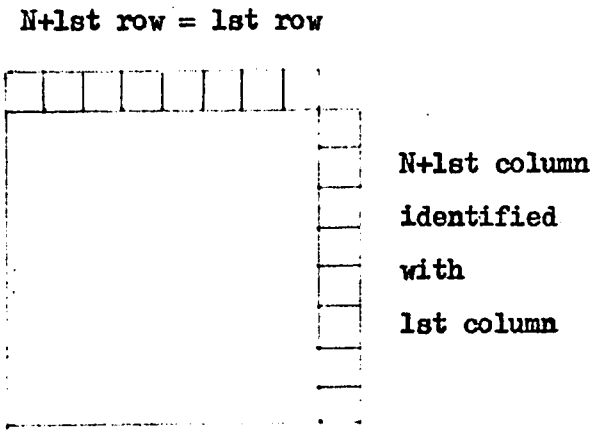


Fig. 1b

We may enumerate the sites by integers (1-dim. models) or by ordered pairs or triplets (2 and 3-dim. models). If periodic boundary conditions exist, one has to introduce appropriate congruences into the scheme of enumeration.

Consider specifically the one dimensional model with N sites. If we denote the spin up, spin down at the k-th site by ± 1, respectively, then the CONFIGURATION of the assembly can be specified by an N-tuplet, $(S_1, \ldots, S_N)$, which in fact is an element of the N-th cartesian power of the set $\{+1,-1\}$:

$$\underline{S} = (S_1, \ldots, S_N) \in \{+1,-1\}^N \quad = (N)$$

and we have 2^N possible configurations. A similar construction is carried out for the models of higher dimension.

To each configuration $\underline{S}$ there corresponds a well defined internal energy of the assembly.

Depending on the mode of interaction between the spins proposed, we can construct a Hamiltonian such that:

$$H(\underline{S}) = \text{configurational energy at } \underline{S}$$

The energy spectrum is therefore discrete and of cardinality not exceeding 2^N. The particles whose spin we have discussed here are localised at the sites and do not have a dynamic state except for vibrations at very high temperatures. This of course is an idealisation for in reality the particles would oscillate about their equilibrium positions at all finite temperatures.

Accordingly, the canonical partition function for an Ising model with N sites is:

$$Z_N = \sum_{\underline{S} \in (N)} \exp(-\beta H(\underline{S})) \qquad (2.1.1)$$

The partition function as a sum of 2^N terms is rather unhandy for evaluation. It is a formidable mathematical task to obtain the closed form solution for Z_N.

For convenience and without loss of generality, we assume the external field as parallel to the spin up direction. Each spin has a potential energy associated with the orientation of its magnetic moment in the field and since we have only two possible orientations, parallel and antiparallel to the field, the spin to field interaction potential at the k-th site can be written as:

$$V(S_k) = -h S_k$$

The constant h is the product of the scalar values of the magnetic moment $\underline{\mu}$ per spin and the external magnetic field $\underline{H}$. The Hamiltonian for the assembly can now be written as:

$$H(\underline{S}) = -h(S_1 + \ldots + S_N) + U(\underline{S}) \qquad (2.1.2)$$

Now $U(\underline{S})$ in (2.1.2) determines the spin to spin interaction potential. The quantity $-\beta H(\underline{S})$ is called the REDUCED ENERGY and on setting $\beta h = c$, we have:

$$Z_N = \sum_{\underline{S} \in (N)} \exp(c(S_1 + \ldots + S_N) - \beta U(\underline{S})) \qquad (2.1.3)$$

The sum $(S_1 + \ldots + S_N)$ is the resultant of the vector sum of the spins and its phase average is called the MAGNETISATION per spin moment, of the assembly. We use the accepted bracket notation:

$$\left\langle \sum_{k=1}^{N} S_k \right\rangle_T = \frac{1}{Z_N} \sum_{\underline{S} \in (N)} \left(\sum_{k=1}^{N} S_k \right) \exp(c \sum_{k=1}^{N} S_k - \beta U(\underline{S}))$$

$$= \frac{\partial}{\partial c} \ln Z_N \quad , \text{ as is seen by inspection.} \qquad (2.1.4)$$

Thus the partition function is a generating function for the magnetisation (as well as for other thermodynamic functions such as internal energy, etc.)

The quantity: $$\left\langle \frac{1}{N} \sum_{k=1}^{N} S_k \right\rangle_T = \frac{\partial}{\partial c} \left(\frac{1}{N} \ln Z_N \right) = m_N(c,T) \qquad (2.1.5)$$

is called the magnetisation per spin and spin moment, it is dimensionless. The assembly is said to be ferromagnetic if in the absence of an external magnetic field and at a certain temperature T_o :

$$m_N(0,T) = 0 \quad , \text{ for } T > T_o$$

$$m_N(0,T) \neq 0 \quad , \text{ for } T < T_o \quad , \quad T_o = \text{CURIE point}$$

The magnetisation as a function of T can be discontinuous at T_o .

The magnetisation per spin and spin moment of a macroscopic assembly is therefore given by the limit:

$$m(c,T) = \lim_{N\to\infty} \frac{\partial}{\partial c} \left(\frac{1}{N} \ln Z_N \right) \qquad (2.1.6)$$

On the other hand, $\lim_{N\to\infty} \left(\frac{1}{N} \ln Z_N \right)$ is frequently easier to evaluate than $\frac{1}{N} \ln Z_N$ by itself, in particular for large values of N .

For convenience we define: $\frac{1}{N} \ln Z_N = G_N$, $\lim_{N\to\infty} G_N = G$

It is therefore important to prove the equality:

$$\frac{\partial}{\partial c} (G) = \lim_{N\to\infty} \frac{\partial}{\partial c} (G_N) \qquad (2.1.7)$$

A sufficient condition for this to hold on a finite interval of the reciprocal temperature 1/T is that:

i) the limit G exists and is uniformly attained,

ii) the partial derivatives are continuous and converge uniformly.

The limit G, as well as its partial derivatives, need not be continuous on all of 1/T , the functions may be piecewise continuous and the CURIE point is possibly a point of discontinuity. As far as our work is concerned, we shall discuss the question of convergence in individual cases when needed.

§ 2) The lattice fluid

Instead of sites we now refer to cells each of which may be occupied, or else empty. We wish to emphasize right here that this changes the viewpoint drastically. When discussing assemblies at an earlier stage, we defined the configuration space as the point set of the simultaneous spatial coordinates of all component systems ; but now we have a lattice whose sites are occupied or else empty. Thus we describe the state of our lattice in terms of the states of the cells and the number of component systems is a p r i o r i variable. A moment of reflection shows that a particular configuration with n component systems present occurs once and only once as the state of the lattice is defined by the N-tuplet:

$$\underline{S} = (S_1, \dots, S_N) \in \{0,1\}^N = (N)$$

That is to say, the correct BOLTZMANN COUNT obtains a p r i o r i !

The configuration space of our lattice represents part of the grand canonical ensemble up to and inclusive N component systems. As we pass to the limit on N, the grand canonical ensemble is exhaustively represented.

The configuration $\underline{S}$ determines the physical state up to an uncertainty in the conjugate momenta of the component systems and there is no way to construct a phase space as the product of configuration space and momentum space. We shall construct an alternate representation.

Let n cells be occupied. Then there are indices k_i , $i = 1, \dots, n$ such that:

$$S_{k_i} = 1 \ , \quad \text{while for} \quad j \neq k_i \ , \quad S_j = 0$$

For such a configuration we have the "inner product" $\underline{S} \cdot \underline{S} = n$, and the inner product gives the total population of the lattice at $\underline{S}$. The power set (N) can now be decomposed into a disjoint union:

$$(N) = \{0,1\}^N = \bigcup_{n=0}^{N} \left\{ \underline{S} \in (N) \ , \ \underline{S} \cdot \underline{S} = n \right\}$$

A phase space can now be constructed as a disjoint union of product sets:

$$\Gamma = \bigcup_{n=0}^{N} W_n \times R^n = \bigcup_{n=0}^{N} \Omega_n \qquad (2.2.1)$$

with R^n from the real line in units of linear momentum and the "unit-step" measure of $W_n = \{ \underline{S} \ , \ \underline{S} \cdot \underline{S} = n \}$ in units of length such that the product :

$$\Delta_n \circ P_1 \circ P_2 \circ \ldots \circ P_n$$

is measured in units of $\hbar^n$, where $\hbar$ is PLANCK's constant and Δ_n is the unit-step measure on W_n. Consider a point $(\underline{S},\underline{P}) \in \Omega_n$. The Hamiltonian has the form:

$$H(\underline{S},\underline{P}) = \frac{1}{2m} (P_1^2 + \ldots + P_n^2) + V(\underline{S}) \qquad (2.2.2)$$

Here P_i is the linear momentum and m is the mass of one component system, whereas $V(\underline{S})$ is the potential energy depending only on $\underline{S}$. The summation of the Boltzmann factor over Ω_n has the form:

$$C \sum_{\underline{S} \in W_n} \exp(-\beta V(\underline{S})) \int_{R^n} \exp\left(- \frac{\beta}{2m} \sum_{k=1}^{n} P_k^2 \right) dP_1 \ldots dP_n$$

which, on evaluation of the multiple integral, becomes:

$$\sum_{\underline{S} \in W_n} \exp(-\beta V(\underline{S}) + \phi \ (\underline{S} \circ \underline{S})) \qquad (2.2.3)$$

Above, C is the constant needed to remove the physical dimension of $\hbar$, that is action, from the partition function. This is done by including C into ϕ, where now:

$$\phi = \frac{1}{2} \ln \left[\frac{2\pi m}{\beta \left[\hbar^2 \right]^\circ} \right] \ , \quad \text{and} \ [\ ]^\circ \text{is to}$$

say that we only retain the physical dimension of the quantity inserted.

Using (2.10) , we have the partition function as the sum:

$$Q_N = \sum_{\underline{S} \in (N)} \exp(-\beta V(\underline{S}) + \phi (\underline{S} \circ \underline{S}))$$

and the grand canonical partition function is the limit on N :

$$Z = \lim_{N \longrightarrow \infty} Q_N$$

We note that no factorial enters into the sum and this is in accordance with our earlier remarks.In the following chapter we shall present a concrete example of the derivation of the closed form partition function based on the methodology derived here.

For 2 or 3-dimensional models we retain the notation (except that $N = M^2$, or $N = M^3$, respectively) and observe that 2 or 3 degrees translational freedom per component system occur.In this case we have:

$$\Gamma = \bigcup_{n=0}^{N} W_n \times R^{fn} \quad , \quad f = 2 \text{ or } 3$$

and then we use:

$$\phi = \frac{f}{2} \ln \left[\frac{2\pi m}{\beta [\hbar^2]^\circ} \right]$$

The Ising model and the lattice fluid have isomorphic configuration spaces, namely the N-th cartesian power of a two element set and the first order interaction models (spin to adjacent spin,cell to adjacent cell) are mathematically equivalent up to an exchange of parameters as this is neatly shown in (I) . The equivalence for models with interaction of higher order is employed in the paper by TROSS and LUND , (II) . The same source also shows the equivalence of a lattice fluid and a ferromagnet,up to exchange of parameters.

Let us return to (2.2.3). The potential energy $V(\underline{S})$ can be written as the sum:

$$V(\underline{S}) = \mu \sum_{k=1}^{N} S_k + U(\underline{S}) \quad , \text{ where } \mu \text{ is the chemical potential per component system and } U(\underline{S}) \text{ is determined by the order of interaction.If we set:}$$

$$c = -\beta\mu + \phi$$

then(2.2.3) can be written as:

$$Q_N = \sum_{\underline{S} \in (N)} \exp\left(c \sum_{k=1}^{N} S_k - \beta U(\underline{S}) \right) \qquad (2.2.4)$$

and: $\sum_{k=1}^{N} S_k = \underline{S} \circ \underline{S}$ = total population of the lattice at $\underline{S}$.

The quantity: (2.2.5)

$$\rho_N = \left\langle \frac{1}{N} \sum_{k=1}^{N} S_k \right\rangle_T = \frac{1}{Q_N} \sum_{\underline{S} \in (N)} \left[\frac{1}{N} \sum_{k=1}^{N} S_k \right] \exp\left(c \sum_{k=1}^{N} S_k - \beta U(\underline{S}) \right)$$

is called the density per component system and component system 's mass, of an assembly having N component systems maximally.The density,as defined by (2.13) is dimensionless and we always have that: $1 \geq \rho_N \geq 0$.

It is seen by inspection that: $\rho_N = \frac{\partial}{\partial c} \left[\frac{1}{N} \ln Q_N \right]$

and if we call: $q_N = \frac{1}{N} \ln Q_N$, $q = \lim_{N \to \infty} q_N$, we have the analogy to the problem of (2.1.7) , § 1 of this chapter.The question has been resolved explicitly for a lattice fluid in the paper by YANG and LEE , see (VI) , and therefore we shall,later on,confine our discussion to:

$$\rho = \frac{\partial}{\partial c} (q) \quad , \text{ for a macroscopic assembly.}$$

CHAPTER III

The derivation by various techniques of the closed form partition function for one dimensional models.

§ 1) The one dimensional lattice fluid. The straight line version.

We demonstrate a simple method of summation over the states for a model with nearest neighbour (first order) interaction potential.

Let $$\underline{S} \in \{0,1\}^N = (N)$$

The potential energy depending on $\underline{S}$ is given by:

$$V(\underline{S}) = \mu \sum_{k=1}^{N} S_k - \eta \sum_{k=2}^{N} S_k S_{k-1}$$

where μ = chemical potential per component system

η = first order interaction potential

We shall use ϕ from (2.2.3), with m being the mass of one particle. For brevity we shall refer to particles rather than to component systems.

Our task is to evaluate the sum:

$$\sum_{\underline{S} \in (N)} \exp(-\beta V(\underline{S}) + \phi (\underline{S} \cdot \underline{S})) = Q_N \qquad (3.1.1)$$

Now $\underline{S} \cdot \underline{S} = S_1 + \dots + S_N = n \quad , \quad 0 \leq n \leq N$

and if we set: $-\mu\beta = u \quad , \quad \phi + u = c \quad , \quad \beta\eta = a \qquad (3.1.2)$

then the sum (3.1.1)

$$\sum_{\underline{S} \in (N)} \exp(c \sum_{k=1}^{N} S_k + a \sum_{k=2}^{N} S_k S_{k-1}) = Q_N \qquad (3.1.3)$$

Next we define : $W_o = \{(S_1, \dots, S_{N-1}, 0)\}$, $W_1 = \{(S_1, \dots, S_{N-1}, 1)\}$

Then it is easy to see that: $W_o \cup W_1 = (N)$, $W_o \cap W_1 = \phi$

Then we take W_1 and define:

$$W_{1o} = \{(S_1, \dots, S_{N-2}, 0, 1)\} , \quad W_{11} = \{(S_1, \dots, S_{N-2}, 1, 1)\}$$

And then again: $$W_{1o} \cup W_{11} = W_1 , \quad W_{1o} \cap W_{11} = \phi$$

The set-theoretic partitioning is now continued in the same spirit and we obtain:

$$(N) = W_o \cup W_{1o} \cup W_{11o} \cup \dots \cup W_{11\dots1o} \cup W_{11\dots11}$$

Thus the summation over (N) can be written as a series of partial sums each of which goes over a disjoint subset of (N).Accordingly,we have:

$$\sum_{(N)} = \sum_{W_o} + \sum_{W_{1o}} + \dots + \sum_{W_{11\dots1o}} + \sum_{W_{11\dots11}}$$

for the summation of the Boltzmann factor (symbolically).

Consider now the subset W_o.The N-th cell is always empty for this set and a short reflection shows that the summation over W_o amounts to Q_{N-1} as defined for arbitrary N by (3.1.3)

Symbolically: $$\sum_{\underline{S} \in W_o} = Q_{N-1} \qquad (3.1.4)$$

Next consider the subset W_{1o}. Here, the N-th cell is always occupied, while the N-1st one is always empty for this set. Observing that the N-th cell does not interact with the remaining N-2 cells, we can "factor out" these two conditions and then we have:

Symbolically:
$$\sum_{\underline{S} \in W_{1o}} = \exp(c)\, Q_{N-2} \qquad (3.1.5)$$

A similar argument shows that for W_{11o}:

$$\sum_{\underline{S} \in W_{11o}} = \exp(2c + a)\, Q_{N-3} \qquad (3.1.6)$$

We continue in this way and obtain finally:

$$\sum_{\underline{S} \in W_{11\ldots1o}} = \exp\left((N-1)c + (N-2)a \right) \qquad (3.1.7)$$

and
$$\sum_{\underline{S} \in W_{11\ldots11}} = \exp\left(Nc + (N-1)a \right)$$

On taking items (3.1.5) to (3.1.7) together, we obtain:

(3.1.8)

$$Q_N = Q_{N-1} + \exp(c)\, Q_{N-2} + \exp(2c + a)\, Q_{N-3} + \ldots$$

$$\ldots + \exp\left((N-1)c + (N-2)a \right) + \exp\left(Nc + (N-1)a \right)$$

This expansion holds for any N sufficiently large to get the expansion started.

We substitute N-1 for N in (3.1.8) ,get a similar expansion which we multiply by exp(c+a) and subtract from this. Upon minor rearrangements, we obtain the recurrence relation:

$$Q_N - (1 + \exp(c+a))\, Q_{N-1} + \exp(c)\,(\exp(a) - 1)\, Q_{N-2} = 0 \qquad (3.1.9)$$

The characteristic polynomial of (3.9) is:

$$p^2 - (1 + \exp(c+a))\, p + \exp(c)\,(\exp(a) - 1) = 0 \qquad (3.1.10)$$

and the roots are:

$$p_{1,2} = \exp\left(\frac{1}{2}(c+a)\right) \cosh\left(\frac{1}{2}(c+a)\right) \pm \sqrt{\exp(c+a)\sinh^2\left(\frac{1}{2}(c+a)\right) + \exp(c)} \qquad (3.1.11)$$

And then,from the theory of recurrence relations,we have the general solution for Q_N :

$$Q_N = A\, p_1^N + B\, p_2^N \qquad (3.1.12)$$

where A and B are determined by substituting two known solutions for Q_k for convenience one would choose $Q_0 = 1$ and $Q_1 = 1 + \exp(c)$.

The coefficients A and B are independent of N . Moreover,we observe that p_1 is the greater one of the two roots.The equation of state in terms of the specific volume v can now be derived.We take the limit:

$$\frac{Pv}{kT} = \lim_{N \to \infty} \frac{1}{N} \ln Q_N = \lim_{N \to \infty} \frac{1}{N} \ln p_1^N + \lim_{N \to \infty} \frac{1}{N} \ln R_N$$

where $R_N = \left[A + \left(\frac{p_2}{p_1}\right)^N B \right]$, and hence $\lim_{N \to \infty} \frac{1}{N} \ln R_N = 0$

Accordingly, we have the equation of state:

$$\frac{Pv}{kT} = \ln p_1 \qquad (3.1.13)$$

It is interesting to inspect the explicit form and to obtain a first approximation for a suitable interval of the temperature T :

$$\frac{Pv}{kT} = \frac{1}{2}(c+a) + \ln\left[\cosh\left(\frac{1}{2}(c+a)\right) + \sqrt{\sinh^2\left(\frac{1}{2}(c+a)\right) + \exp(-a)}\right]$$

Consider an interval of T such that $\left|\sinh\left(\frac{1}{2}(c+a)\right)\right| >> 1$

Then we have to a first approximation:

$$\frac{Pv}{kT} \cong c + a = \frac{1}{2}\ln\left[\frac{2\pi mkT}{[h^2]^\circ}\right] + \frac{\eta - \mu}{kT}$$

On using the thermodynamic relations stated and proved in (I), Chapter 8, we can show that the mean energy per particle is given by:

$$u(T) \cong \frac{kT}{2} + \mu - \eta$$

and accordingly, the specific heat is:

$$C_v \cong \frac{k}{2} \quad \text{, per particle}$$

Furthermore, on using the first approximation, we can show that the mean kinetic energy per particle is:

$$\text{k.e.} \cong \frac{kT}{2}$$

On noting that the assembly has only one degree of linear freedom per particle, we see that the results agree with the known thermodynamic data of an ideal gas.

As discussed in § 2 of chapter II , the density per particle and particle mass is given by:

$$\rho(\eta, \mu, T) = \frac{\partial}{\partial c} \left[\lim_{N \to \infty} \frac{1}{N} \ln Q_N \right] = \frac{\partial}{\partial c} \ln p_1$$

so that:

$$\rho(\eta, \mu, T) = \frac{1}{2} \left\{ 1 + \frac{\sinh\left(\frac{1}{2}(c+a)\right)}{\sqrt{\sinh^2\left(\frac{1}{2}(c+a)\right) + \exp(-a)}} \right\} \qquad (3.1.14)$$

We consider the density for the chemical standard state , that is $\mu = 0$, see for example (V),page 205 . Furthermore,we shall confine ourselves to temperatures

$$T \ll \left[\frac{[\hbar^2]^\circ}{2\pi mk} \right] \approx \frac{10^{16}}{m}$$

(this remark will be repeated in § 5 of this chapter , but in a somewhat different context) . This is a realistic upper bound.

Hence: $$\frac{1}{2} \ln \left[\frac{2\pi mkT}{[\hbar^2]^\circ} \right] \ll -1 \qquad (3.1.15)$$

and therefore: $$\sinh\left(\frac{1}{2} \left[\frac{\nu}{kT} + \frac{1}{2} \ln \left[\frac{2\pi mkT}{[\hbar^2]^\circ} \right] \right] \right) \ll 0$$

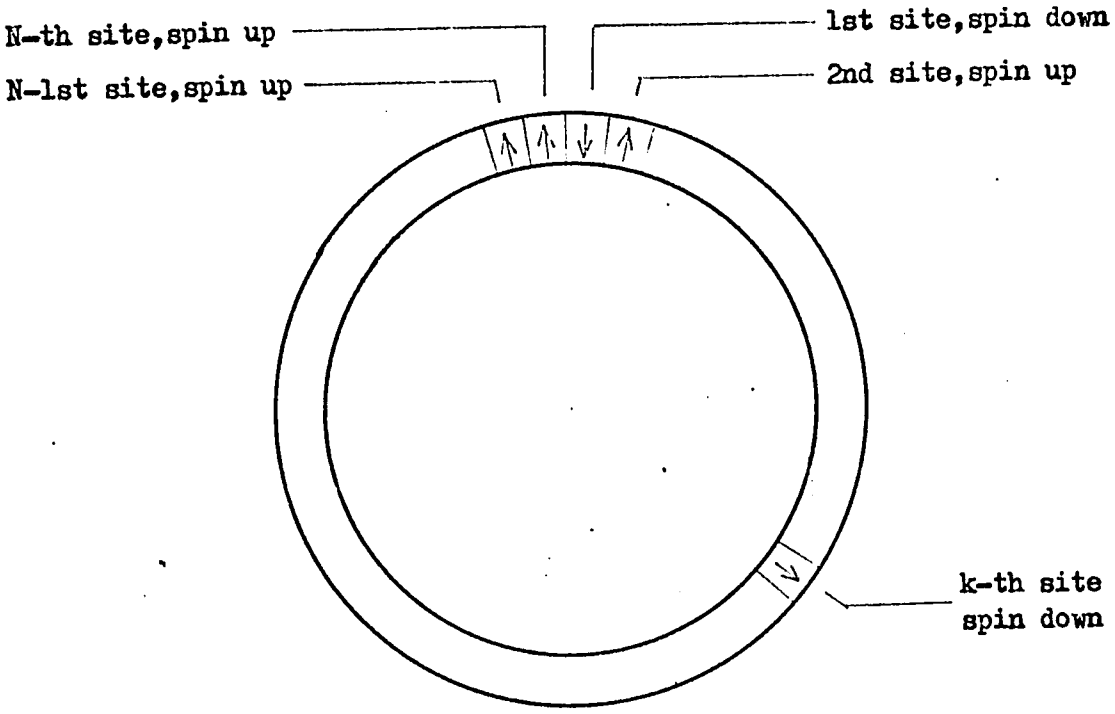
whence: $\rho(\eta, 0, T) \approx 0$, for $T \approx \frac{10^{10}}{m}$, say .

On the other hand it is seen by inspection that : $\lim_{T \to 0} \rho(\eta, 0, T) = 1$

and for,say $\frac{10^{10}}{m} > T > 0$, ρ varies continuously.Similarly, all the other thermodynamic function will vary continuously and the model exhibits no critical phenomenon.In § 5 of this chapter we shall show the possibility of phase change for this model as the potential is modified.

§ 2) The Ising ring.Exact statistics for second order interactions.

We consider the ring model with an even number of sites, $N = 2M$, and identify the pair of sites (N+1,N+2) with the pair (1,2) and our enumeration is therefore modulo N.The magnetic field,if present,is perpendicular to the plane on which the ring lies.



Spin up,drawn outward here,means parallel to the normal of the plane (and hence parallel to the magnetic field,if present) and spin down, drawn inward,means antiparallel to the normal.Our model has a second order interaction potential:

$$-\nu S_k S_{k-2}$$

in addition to the first order interaction potential and spin to field potential given by:

$$-\eta S_k S_{k-1} \text{ , and } -hS_k \text{ , respectively.}$$

Accordingly, the Hamiltonian is given as:

$$H(\underline{S}) = -h \sum_{k=1}^{N} S_k - \eta \sum_{k=1}^{N} S_k S_{k-1} - \nu \sum_{k=1}^{N} S_k S_{k-2}$$

and the congruence modulo N must be applied to indices with non-positive or zero value. Let us substitute:

$$\eta\beta = a \quad , \quad \nu\beta = b \quad , \quad \beta h = c$$

The reduced energy can now be written as the sum:

$$-\beta H(\underline{S}) = \sum_{k=1}^{M} \left[c(S_{2k-1} + S_{2k}) + a(S_{2k-1}S_{2k} + S_{2k}S_{2k+1}) + b(S_{2k-1}S_{2k+1} + S_{2k}S_{2k+2}) \right]$$

where our enumeration modulo N is kept in mind as well as our initial provision that $N = 2M$. The Boltzmann factor can now be written as a product:

$$\exp(-\beta H(\underline{S})) = \prod_{k=1}^{M} (S_{2k-1}, S_{2k} \mid R \mid S_{2k+1}, S_{2k+2}) \qquad (3.2.1)$$

where:

$$(S_{2k-1}, S_{2k} \mid R \mid S_{2k+1}, S_{2k+2}) = \exp(c(S_{2k-1} + S_{2k}) + \dots)$$

Consequently, the partition function is the sum:

$$(3.2.2)$$

$$Q_N = \sum_{\underline{S} \in (N)} \prod_{k=1}^{M} (S_{2k-1}, S_{2k} \mid R \mid S_{2k+1}, S_{2k+2})$$

Let us put into one-one correspondence:

$$\underline{S} = (S_1, S_2, \dots, S_{N-1}, S_N) \longleftrightarrow (S''_1, \dots, S''_M) = \underline{S}'' \qquad (3.2.3)$$

with:

$$S''_k = (S_{2k-1}, S_{2k}) \in \{+1, -1\}^2$$

Actually, the correspondence (3.2.4) is obvious since we have the set-theoretical equivalence:

$$(N) = \{+1,-1\}^N \hat{=} \left\{\{+1,-1\}^2\right\}^M \qquad (3.2.4)$$

If we agree to order $\{+1,-1\}$ by : $+1 \prec -1$, then $\{+1,-1\}^2$ has the induced order after first differences: $(1,1) \prec \ldots \prec (-1,-1)$.

Accordingly, S''_k assumes 4 well ordered values. In view of the set equivalence above we can now write:

$$Q_N = \sum_{S''_1, \ldots, S''_M \in \{+1,-1\}^2} \prod_{k=1}^{M} (S''_k \mid R \mid S''_{k+1})$$

That is:

$$Q_N = \text{Trace } \underline{R}^M .$$

where $\underline{R}$ is a well defined 4 x 4 matrix which we have tabulated (table I). It is seen that $\underline{R}$ is not symmetric. Furthermore, $\underline{R}$ can be written as the product of two matrices:

$$\underline{R}(c,a,b) = \underline{H}(c) \circ \underline{A}(a,b)$$

which can be seen in table II . The matrix $\underline{A}$ is not symmetric.

A sufficient condition for the diagonalisation of $\underline{R}$ is that its eigenvalues be distinct. If this is found to be true, then:

$$Q_N = \lambda_1^M + \ldots + \lambda_4^M \qquad (3.2.5)$$

The λ_i , $i = 1,2,3,4$ are the eigenvalues of the matrix $\underline{R}$. The expression (3.2.5) is then the sought closed-form solution for the partition function.

Table I

The matrix $\underline{R}$:

$$\begin{bmatrix} \exp(2c+2a+2b) & \exp(2c+2a) & \exp(2c) & \exp(2c-2b) \\ \exp(-2a) & \exp(-2a+2b) & \exp(-2b) & 1 \\ 1 & \exp(-2b) & \exp(-2a+2b) & \exp(-2a) \\ \exp(-2c-2b) & \exp(-2c) & \exp(-2c+2a) & \exp(-2c+2a+2b) \end{bmatrix}$$

Table II

The product: $\underline{R}(c,a,b) = \underline{H}(c) \cdot \underline{A}(a,b)$

$$\begin{bmatrix} \exp(2c) & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & \exp(-2c) \end{bmatrix} \begin{bmatrix} \exp(2a+2b) & \exp(2a) & 1 & \exp(-2b) \\ \exp(-2a) & \exp(2b-2a) & \exp(-2b) & 1 \\ 1 & \exp(-2b) & \exp(2b-2a) & \exp(-2a) \\ \exp(-2b) & 1 & \exp(2a) & \exp(2a+2b) \end{bmatrix}$$

We wish to point out that: $\mathrm{Det}(\underline{R}) = \mathrm{Det}(\underline{H}).\mathrm{Det}(\underline{A}) = \mathrm{Det}(\underline{A})$ and hence the product of the anticipated eigenvalues is independent of c .Therefore,the product of the eigenvalues is independent of the scalar value of the magnetic field.

We inspect the matrix $\underline{A}$ a bit closer. It is seen that $\underline{A}$ can be written in terms of 2 x 2 submatrices $\underline{W}$ and $\underline{U}$:

$$\underline{A} = \begin{bmatrix} \underline{U} & \underline{W} \\ \underline{W} & \underline{XUX} \end{bmatrix} \qquad (3.2.6)$$

where $\underline{X}$ is the first PAULI spinor:

$$\underline{X} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} , \quad \text{and} \quad \underline{X}^2 = \underline{I} , \quad 2 \times 2 \text{ unit matrix.}$$

We construct a similarity transformation on $\underline{R}$ which subsequently acts on $\underline{H}$ and $\underline{A}$. The transformation is effected by the matrix $\underline{D}$:

$$\underline{D} = \frac{1}{\sqrt{2}} \begin{bmatrix} \underline{I} & +\underline{X} \\ -\underline{X} & \underline{I} \end{bmatrix}$$

and:

$$\underline{D}^{-1} = \frac{1}{\sqrt{2}} \begin{bmatrix} \underline{I} & -\underline{X} \\ +\underline{X} & \underline{I} \end{bmatrix} \qquad (3.2.7)$$

The results of the similarity transformation on $\underline{H}$ and $\underline{A}$ are given in table III .

It is quite interesting to note in passing that the transformed $\underline{H}$, call it $\underline{H}'$, is a LORENTZ matrix, corresponding to a frame moving with the uniform velocity v along x_1 , where:

$$v = C \tanh 2c , \qquad C = \text{velocity of light.}$$

We do not wish to speculate at this time on the physical relevance of this observation.

On setting $c = 0$, the matrix $\underline{H}$ turns into the 4 x 4 unit matrix.

$$\underline{H}(0) = \underline{I}_{4x4}$$

Table III

i) The matrix $\underline{A}' = \underline{D} \cdot \underline{A} \cdot \underline{D}^{-1}$:

$$2 \begin{bmatrix} \exp(a)\cosh(2b+a) & \exp(a)\cosh(a) & \multicolumn{2}{c}{\multirow{2}{*}{ZERO}} \\ \exp(-a)\cosh(a) & \exp(-a)\cosh(2b-a) & & \\ \multicolumn{2}{c}{\multirow{2}{*}{ZERO}} & \exp(-a)\sinh(2b-a) & -\exp(-a)\sinh(a) \\ & & \exp(a)\sinh(a) & \exp(a)\sinh(2b+a) \end{bmatrix}$$

ii) The matrix $\underline{H}' = \underline{D} \cdot \underline{H} \cdot \underline{D}^{-1}$:

$$\begin{bmatrix} \cosh(2c) & 0 & 0 & -\sinh(2c) \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ -\sinh(2c) & 0 & 0 & \cosh(2c) \end{bmatrix}$$

We see by inspection that: $\underline{H}(0) = I_{4x4}$

We state the well known fact that the similarity transformation leaves the characteristic polynomial and hence the eigenvalues unchanged. The matrix $\underline{A}'$ is multiplied by 2 so that the determinant is multiplied by 16. The determinant of the entire product has the value : $16 \sinh^4 2b$.

Thus on setting $c = 0$, the characteristic polynomial resolves into two quadratic equations which we solve and the two sets of roots are:

$$\overset{o}{\lambda}_{1,2} = \exp(2b)\cosh 2a + \exp(-2b) \pm \sqrt{(\exp(2b)\cosh 2a + \exp(-2b))^2 - 4\sinh^2 2b}$$

and: (3.2.8)

$$\overset{o}{\lambda}_{3,4} = \exp(2b)\cosh 2a - \exp(-2b) \pm \sqrt{(\exp(2b)\cosh 2a - \exp(-2b))^2 - 4\sinh^2 2b}$$

corresponding to the upper left and lower right submatrix, respectively. The eigenvalues are seen to be distinct and consequently we have :

$$Q_N(0,a,b) = \overset{o\ M}{\lambda}_1 + \ldots + \overset{o\ M}{\lambda}_4 \qquad (3.2.9)$$

We proceed to obtain the characteristic polynomial for the general case where $c \neq 0$. The expansion of the eigenvalue equation is conveniently done in accordance with the following theorem:

THEOREM : For $0 \leq r < n$, the coefficient of λ^r in the characteristic polynomial of an $n \times n$ matrix $\underline{M}$ is equal to $(-1)^{n-r}$ times the sum of all $(n-r)$-rowed principal minors of $\underline{M}$.

The theorem is quoted from (III), page 197. Hence we must solve a 4-th degree equation. On performing the expansion, we obtain the equation:

$$\begin{aligned} \lambda^4 &- 2\lambda^3 \exp(2b)(\exp(2a)\cosh 2c + \exp(-2a)) \\ &+ \lambda^2 (4\cosh 2c(\exp(4b) - 1) + 2(\exp(4b)\cosh 4a - \exp(-4b))) \\ &- 8\lambda \exp(2b)(\exp(-2a)\cosh 2c + \exp(2a))\sinh^2 2b \\ &+ 16\sinh^4 2b = 0 \end{aligned} \qquad (3.2.10)$$

The equation (3.2.1o) is difficult to solve. We rewrite it in the form:

$$\lambda^4 - 2\lambda^3 \exp(2b)(\exp(2a)\cosh 2c + \exp(-2a)) \qquad (3.2.11)$$

$$+ \lambda^2 (4\cosh 2c(\exp(4b)-1) + 2(\exp(4b)\cosh 4a - \exp(-4b)))$$

$$- 8\lambda \exp(2b)(\exp(2a)\cosh 2c + \exp(-2a)) \sinh^2 2b$$

$$+ 16 \sinh^4 2b = 8\lambda \exp(2b)(\cosh 2c - 1)\sinh 2a \sinh^2 2b$$

Then it is seen that the right side can be made as small as we please, if we confine our considerations to a finite interval of the reciprocal temperatur 1/T and take c sufficiently small. For further brevity, we rewrite (3.2.11) as:

$$L(\lambda) = \Delta_0 \lambda \ , \quad \text{where} \quad \Delta_0 \longrightarrow 0 \quad \text{as} \quad c \longrightarrow 0$$

Next let ζ_i , $i = 1,2,3,4$, be the four roots of $L(\zeta) = 0$. These roots are distinct, as we shall see, that is there are no repeated roots.

Moreover:

for any $\epsilon > 0$, we can find a $\delta > 0$

such that $|\lambda_i - \zeta_i| < \epsilon$ whenever $c < \delta$ (3.2.12)

It follows that we have:

$$\left.\begin{aligned} \lambda^3 &= \zeta^3 + \Delta_3 \\ \lambda^2 &= \zeta^2 + \Delta_2 \\ \lambda &= \zeta + \Delta_1 \end{aligned}\right\} \quad \Delta_i \longrightarrow 0 \ , \text{ as } c \longrightarrow 0$$

$$\lambda^4 = \zeta^4 + \Delta_4 \qquad (3.2.12a)$$

Denote by primes the differentiation with respect to c.Furthermore, let e , f , g be the coefficients of λ^3 , λ^2 and λ ,respectively. We consider the equation:

$$[L(\lambda)]' - [L(\zeta)]' = \Delta_0'\lambda + \Delta_0\lambda'$$

and on writing it out,we obtain:

$$\begin{aligned}(\lambda' - \zeta')(4\zeta^3 + 3\zeta^2 e + 2\zeta f + g) \\ - \lambda'(4\Delta_3 + 3\Delta_2 e + 2\Delta_1 f) \\ + \Delta_3 e' + \Delta_2 f' + \Delta_1 g' \\ = \Delta_0'\lambda + \Delta_0\lambda'\end{aligned} \qquad (3.2.13)$$

Consequently,on taking the limit on c :

$$\lim_{c \to 0} (\lambda' - \zeta')(4\zeta^3 + 3\zeta^2 e + 2\zeta f + g) = 0$$

But the right bracket is seen to be the derivative of $L(\zeta)$ with respect to ζ and there are no repeated roots.Hence ζ is not a root of the cubic equation in the bracket and therefore:

$$\lim_{c \to 0} (\lambda' - \zeta') = 0 \qquad (3.2.14)$$

We have shown that: $\lim_{c \to 0} \lambda' = \lim_{c \to 0} \zeta'$

Now let λ_i be the four roots of (3.2.11) :

$$L(\lambda) = \Delta_o \lambda \qquad (3.2.15)$$

for small c . The partition function is given by:

$$Q_N = \lambda_1^M + \dots + \lambda_4^M \qquad (3.2.16)$$

The greatest root of (3.2.11) have the index 1 , and we set $\lambda_1 = \Delta$

Furthermore,denote by r_i , $i = 2,3,4$, the three ratios:

$$\frac{\lambda_i}{\Delta} = r_i < 1 \qquad (3.2.17)$$

and consider:

$$q_N = \frac{1}{N} \ln Q_N = \frac{1}{2M} \ln \left[\Delta^M (1 + r_2^M + r_3^M + r_4^M) \right]$$

so that:

$$\lim_{N \to \infty} q_N = \frac{1}{2} \ln \Delta = q \qquad (3.2.18)$$

The limit attains uniformly as the following argument shows:

$$\left| q - q_N \right| = \left| \frac{1}{N} \ln (1 + \dots + r_4^M) \right|$$

$$\leq \frac{1}{N} \ln 4 < \epsilon$$

whenever $N > \frac{\ln 4}{\epsilon}$. QED . Thus the first of the two conditions is satisfied.It remains to discuss the convergence of the derivatives.

Denote by primes differentiation with respect to c :

$$q'_{2k} = \frac{\Lambda'}{2\Lambda} + \frac{1}{2}\left[\frac{r_2^{k-1}r_2' + \dots + r_4^{k-1}r_4'}{1 + \dots + r_4^{k}}\right]$$

for an integer k and similarly for an integer j . Consider an interval of $\frac{1}{T}$ not containing zero and bounded above.None of the roots of (3.2.11) has a zero on such an interval (this follows from $16 \sinh^4 2b = \lambda_1 \circ \dots \circ \lambda_4$) Hence the derivatives of the ratios r_i remain bounded on such an interval. Therefore,let n_i be the constants such that $r_i' \leqq n_i$, and let n be the greatest of the n_i , then $r_i' \leqq n$ .For the ratios themselves we have constants $m_i < 1$, such that $r_i < m_i$ on said interval and we denote by m the greatest m_i .

Denote the bilinear fraction in q_{2k} above by R_{2k} . Then it is seen by inspection that:

$$\lim_{k \to \infty} R_{2k} \leqq \lim_{k \to \infty} m^{k-1} n = 0 \text{ , uniformly.}$$

Therefore,as R_{2k} coverges uniformly to zero , q'_{2k} converges uniformly.

We have shown that:

$$\frac{\partial}{\partial c}\left[\lim_{N \to \infty} \frac{1}{N} \ln Q_N\right] = \lim_{N \to \infty}\left[\frac{\partial}{\partial c} \frac{1}{N} \ln Q_N\right]$$

so that:

$$m(0,T) = \lim_{c \to 0} \frac{\Lambda'}{2\Lambda} \qquad (3.2.19)$$

In view of (3.2.12a),(3.2.14)we are in a position to replace (3.2.19) by :

$$m(0,T) = \lim_{c \to 0} \frac{\zeta'_m}{2\zeta_m} \qquad (3.2.20)$$

where ζ_m is the greatest of the roots of $L(\zeta) = 0$, see (3.2.11)

It remains to solve that equation.The equation can be resolved into two quadratic factors:

$$(\zeta^2 + p_1\zeta + 4\sinh^2 2b)(\zeta^2 + p_2\zeta + 4\sinh^2 2b) \qquad (3.2.21)$$

where $p_{1,2}$ have the somewhat awkward form:

$$p_{1,2} = -\exp(2b)(\exp(2a)\cosh 2c + \exp(-2a))$$
$$\pm \Big[\exp(4b)(\exp(2a)\cosh 2c + \exp(-2a))^2 - 4\cosh 2c(\exp(4b) - 1)$$
$$-2(\exp(4b)\cosh 4a - \exp(-4b)) + 8\sinh^2 2b\Big]^{\frac{1}{2}} \qquad (3.2.22)$$

Accordingly we have:

$$\zeta_m = -\frac{1}{2}\left(p_2 - \sqrt{p_2^2 - 16\sinh^2 2b}\right)$$

It is seen by inspection that: $\zeta_m = \zeta_m(\cosh 2c, a, b)$, and hence :

$$\zeta'_m = \left[\frac{\partial \zeta_m}{\partial(\cosh 2c)}\right] \sinh 2c \cdot 2 \qquad (3.2.23)$$

A separate calculation, which we forego, would show that none of the surds involved has a zero at $c = 0$.(for finite and non-zero T)

Hence from (3.2.23) :

$$\lim_{c \to 0} \zeta'_m = 0$$

On the other hand, from (3.19):

$$\lim_{c \to 0} \zeta_m \neq 0$$

and therefore:

$$m(0,T) = 0$$

for all finite and non-zero temperatures. The model does not exhibit ferromagnetic behaviour.

The free energy f of a macroscopic assembly was given by:

$$f = \lim_{N \to \infty} \frac{1}{N} \ln Q_N$$

$$= \frac{1}{2} \ln \Lambda$$

For sufficiently small c we have to a good approximation:

$$f \doteq \frac{1}{2} \ln \zeta_m$$

and we can derive other thermodynamic functions from this.

§ 3 Extension of the matrix method to interactions of higher order

We continue to discuss the ring model. Let $\eta_1, \eta_2, \cdots, \eta_r$ be the interaction potentials between the spins separated by the "distance" 1,2 and r, respectively. Furthermore, we require that $N = Mr$, so that N is a composite number. The justification for this provision will become apparent as we go on. In order to avoid "self-interaction" terms, we must have $M > r$.

Let: $\underline{S} \in (N)$. Set $\beta\eta_i = a_i$, for $i = 1,2, \cdots, r$, $\beta h = c$.

The reduced Hamiltonian has the form:

$$-\beta H(\underline{S}) = c \sum_{k=1}^{N} S_k + a_1 \sum_{k=1}^{N} S_k S_{k+1} + \cdots + a_r \sum_{k=1}^{N} S_k S_{k+r} \qquad (3.3.1)$$

In view of our initial provision that $N = rM$:

$$-\beta H(\underline{S}) = \sum_{k=1}^{M} \Bigg[c \sum_{j=1}^{r} S_{(k-1)r+j} + a_1 \sum_{j=1}^{r} S_{(k-1)r+j} S_{(k-1)r+j+1} \qquad (3.3.2)$$

$$+ \cdots + a_r \sum_{j=1}^{r} S_{(k-1)r+j} S_{kr+j} \Bigg]$$

and we write for brevity: $$-\beta H(\underline{S}) = \sum_{k=1}^{M} \sum(k,r) \qquad (3.3.3)$$

where $\sum(k,r)$ is that part of the reduced Hamiltonian which depends only on the two r-tuplets $(S_{(k-1)r+1}, \cdots, S_{kr})$ and $(S_{kr+1}, \cdots, S_{(k+1)r})$.

In view of the periodic boundary conditions:

$$(S_{Mr+1}, \cdots, S_{(M+1)r}) = (S_1, \cdots, S_r) \qquad (3.3.4)$$

In view of the set-theoretical equivalence discussed before, we have:

$$Q_N = \sum_{\underline{S} \in (N)} \exp(-\beta H(\underline{S})) = \sum_{S_1^r, S_2^r, \ldots, S_M^r \in \{+1,-1\}^r} \prod_{k=1}^{M} (S_k^r \mid R \mid S_{k+1}^r) \qquad (3.3.7)$$

That is to say:

$$Q_N = \text{Trace } \underline{R}^M$$

where $\underline{R}$ is a well defined $2^r \times 2^r$ matrix whose elements are given by:

$$(S_k^r \mid R \mid S_{k+1}^r) = \exp(\sum(k,r)) \qquad (3.3.8)$$

see (3.3.2) and (3.3.3) . The matrix $\underline{R}$ is not symmetric. If this matrix can be diagonalised, then:

$$Q_N = \lambda_1^M + \ldots + \lambda_{2^r}^M \qquad (3.3.9)$$

where the λ_i are the eigenvalues of $\underline{R}$. We inspect the matrix $\underline{R}$ whose elements are given by (3.3.8) above. On inspecting the sums in the exponential , see (3.3.2) , we note that: $c \sum_{j=1}^{r} S_{(k-1)r+1}$

is constant on rows, that is it depends only on S_k^r and accordingly we can write $\underline{R}$ as a product of two matrices one of which is diagonal:

$$\underline{R}(c, a_1, \ldots, a_r) = \underline{H}(c) \circ \underline{A}(a_1, \ldots, a_r) \qquad (3.3.10)$$

where:

$$\underline{H}(c) = \text{Diagonal } \left[\exp(rc), \exp((r-2)c), \ldots, \exp(-rc)\right]$$

The Boltzmann factor can now be written as a product:

$$\exp(-\beta H(\underline{S})) = \prod_{k=1}^{M} \exp\Big(\sum (k,r) \Big)$$

$$= \prod_{k=1}^{M} (S_{(k-1)r+1}, \cdots, S_{kr} \mid R \mid S_{kr+1}, \cdots, S_{(k+1)r}) \qquad (3.3.5)$$

As we sum for the partition function: $Q_N = \sum_{\underline{S} \in (N)} \exp(-\beta H(\underline{S}))$

$\underline{S}$ may run in an arbitrary order through (N) . Let us put into one-one correspondence:

$$(S_1, S_2, \cdots, S_r, \cdots, S_{(M-1)r+1}, S_{(M-1)r+2}, \cdots, S_{Mr}) \longleftrightarrow (S_1^r, \cdots, S_M^r)$$

where: $S_j^r = (S_{(j-1)r+1}, \cdots, S_{jr})$ for $j = 1,2, \cdots, M$

The above one-one correspondence is a consequence of the set-theoretical equivalence:

$$\{+1,-1\}^N = \{\{+1,-1\}^r\}^M$$

since $N = rM$. If we order $\{+1,-1\}$ by $+1 \prec -1$,

Then $\{+1,-1\}^r$ is ordered after first differences:

$$(1, \cdots, 1) \prec (1, \cdots, 1, -1) \prec \cdots \prec (-1, \cdots, -1) \qquad (3.3.6)$$

The set $\{+1,-1\}^r$ has 2^r elements, r-tuplets, that is, and for each $j=1,2,\cdots,M$ $S_j^r \in \{+1,-1\}^r$, and because of (3.3.6) , the S_j^r have a definite order.

The matrix $\underline{A}$, which is not symmetric, is given by: $(S_k^r \mid A \mid S_{k+1}^r) =$

$$= \exp\left[a_1 \sum_{j=1}^{r} S_{(k-1)r+j} S_{(k-1)r+j+1} + \dots + a_r \sum_{j=1}^{r} S_{(k-1)r+j} S_{kr+j} \right] \qquad (3.3.11)$$

We note that: $$(-S_k^r \mid A \mid -S_{k+1}^r) = (S_k^r \mid A \mid S_{k+1}^r) \qquad (3.3.12)$$

and this is a rather useful symmetry, the importance of which becomes apparent after our:

LEMMA (3.3.13) : Let $\{+1,-1\}^r = (r)$ be the r-th cartesian power of the set $\{+1,-1\}$, which is ordered by $+1 \prec -1$. If $\underline{S}_p \in (r)$ is the p-th element of (r) with $1 \leq p \leq 2^{r-1}$,

then $-\underline{S}_p$ is the $(2^r + 1 - p)$-th element of (r).

Proof: We proceed by induction on p . Let us create a correspondence by defining:

$$\phi : \quad (r) \longrightarrow (r)$$

such that:

$$\phi(\underline{S}_p) = -\underline{S}_p$$

then clearly ϕ maps the first element into the last one, that is the 2^r- th .

$$\phi((1, \dots ,1)) = (-1, \dots , -1)$$

and our assertion holds good for $p = 1$. Now let ϕ take the the p - th element into the $(2^r + 1 - p)$-th one. Consider the p+1st element of (r) and compare them to the possible extend:

$\underline{S}_p = (1, \dots ,1,1, \dots)$, and because of our first difference ordering:

$$\underline{S}_{p+1} = (1, \dots ,1,-1, \dots)$$

Then we have that: $\phi(\underline{S}_{p+1}) = (-1, \ldots, -1, 1, \ldots)$

and: $\phi(\underline{S}_{p}) = (-1, \ldots, -1, -1, \ldots)$

and therefore: $\phi(\underline{S}_{p+1}) \prec \phi(\underline{S}_{p})$ since (r) is ordered after first differences. A moment of reflection shows that the images of consecutive elements are consecutive - the order being reversed. Therefore, by induction:

$$\phi(\underline{S}_{1}) = \underline{S}_{2^r}$$

$$\phi(\underline{S}_{2}) = \underline{S}_{(2^r - 1)}$$

$$\vdots$$

$$\phi(\underline{S}_{2^{r-1}}) = \underline{S}_{(2^{r-1} + 1)} \qquad \text{QED.}$$

Remark: For the sake of clarity we took elements with a row of consecutive ones preceding the first difference. In general, the row preceding the first difference is arbitrary. The row following the first difference is determined by the ordinal number p and is merely multiplied by -1 as we pass from $\underline{S}_{p}$ to its image under ϕ.

Now let S_k^r and S_{k+1}^r be the p - th and the q - th element of $\{+1,-1\}^r$, respectively. Then in view of our lemma : (for $1 \leq p,q \leq 2^{r-1}$)

$$A_{p,q} = A_{(2^r + 1 - p),(2^r + 1 - q)} \qquad (3.3.14)$$

and the obvious variation:

$$A_{p,(2^{r-1} + 1 - q)} = A_{(2^r + 1 - p),(2^{r-1} + q)} \qquad (3.3.14a)$$

as well as: $A_{p,(2^r+1-q)} = A_{(2^r+1-p),q}$ (3.3.14b)

Next consider the $2^{r-1} \times 2^{r-1}$ submatrix $\left[A_{p,q}\right]$ of $\underline{A}$. By what we just have proved, each element of $\left[A_{p,q}\right]$ is also found in the $2^{r-1} \times 2^{r-1}$ submatrix $\left[A_{(2^r+1-p),(2^r+1-q)}\right]$ of $\underline{A}$, for $1 \leq p,q \leq 2^{r-1}$

This follows from item (3.3.14). Let us change the column/row indexing of the submatrix $\left[A_{(2^r+1-p),(2^r+1-q)}\right]$, now going from $2^{r-1}+1$ to 2^r, to j,k with $1 \leq j,k \leq 2^{r-1}$, and call the so redefined submatrix $\left[B_{j,k}\right]$.

Then by virtue of (3.3.14): $A_{p,q} = B_{(2^{r-1}+1-p),(2^{r-1}+1-q)}$

and also:

$$B_{p,q} = A_{(2^{r-1}+1-p),(2^{r-1}+1-q)}$$

for: $1 \leq p,q \leq 2^{r-1}$. We can construct the matrix product:

$$B_{j,k} = \sum_{p,q} \Omega_{j,p} A_{p,q} \Omega_{q,k} \qquad (3.3.14c)$$

where: $\Omega_{j,p} = \delta_{(2^{r-1}+1-j),p}$ is a symmetric $2^{r-1} \times 2^{r-1}$ matrix, and δ is the Kronecker delta. The matrix $\underline{\Omega} = \left[\Omega_{p,q}\right]$ is in fact the r-1st Kronecker product of the first Pauli spinor:

$$\underline{\Omega} = \underline{X} \circledast \underline{X} \circledast \cdots \circledast \underline{X}, \text{ where: } \underline{X} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

It is seen by inspection that: $\underline{\Omega}^2 = I_{2^{r-1} \times 2^{r-1}}$

Hence: $\left[A_{(2^r+1-p),(2^r+1-q)}\right] = \left[B_{j,k}\right] = \underline{\Omega}\left[A_{p,q}\right]\underline{\Omega}$.

Next we consider the submatrices $\left[A_{p,(2^r+1-q)}\right]$, $\left[A_{(2^r+1-p),q}\right]$ of $\underline{A}$. (for $1 \leq p,q \leq 2^{r-1}$)

Let us consider item (3.3.14b) : $A_{p,(2^r+1-q)} = A_{(2^r+1-p),q}$

On the left side, the row index goes from $2^{r-1}+1$ to 2^r , and similarly for the column index on the right side. In the same spirit as before, we replace (2^r+1-p) by k , and (2^r+1-q) by j , where: $1 \leq j,k \leq 2^{r-1}$. Then we define matrices $\underline{B}^1$ and $\underline{B}^2$ by: (for $1 \leq p,q,j,k \leq 2^{r-1}$)

$$\left[B^1_{p,j}\right] = \left[A_{p,(2^r+1-q)}\right] , \left[B^2_{k,q}\right] = \left[A_{(2^r+1-p),q}\right]$$

Then (3.3.14b) , stated above , amounts to:

$$B^1_{p,(2^{r-1}+1-j)} = B^2_{(2^{r-1}+1-p),j}$$

and on setting : $k = 2^{r-1}+1-j$, we have $1 \leq k \leq 2^{r-1}$, and also:

$$B^1_{p,k} = B^2_{(2^{r-1}+1-p),(2^{r-1}+1-k)}$$

In analogy to (3.3.14c) , we construct the matrix product:

$$B^1_{p,k} = \sum_{j,q} \Omega_{p,j} \; B^2_{j,q} \; \Omega_{q,k} \qquad (3.3.14d)$$

and therefore: $\left[A_{p,(2^r+1-q)}\right] = \underline{\Omega}\left[A_{(2^r+1-p),q}\right]\underline{\Omega}$

Let us consider the upper two submatrices of $\underline{A}$, and define:

$$\left[A_{p,q} \right] = \underline{U} \quad , \quad \text{and} \quad \left[A_{p,(2^r + 1 - q)} \right] = \underline{W}$$

then $\underline{A}$ can be written in terms of these two submatrices alone, that is:

$$\underline{A} = \begin{bmatrix} \underline{U} & \underline{W} \\ \underline{\Omega}\,\underline{W}\,\underline{\Omega} & \underline{\Omega}\,\underline{U}\,\underline{\Omega} \end{bmatrix} \qquad (3.3.15)$$

We construct a similarity transformation:

$$\underline{D} = \frac{1}{\sqrt{2}} \begin{bmatrix} I & +\underline{\Omega} \\ -\underline{\Omega} & I \end{bmatrix} \quad , \quad \underline{D}^{-1} = \frac{1}{\sqrt{2}} \begin{bmatrix} I & -\underline{\Omega} \\ +\underline{\Omega} & I \end{bmatrix} \qquad (3.3.16)$$

then it can be verified that: (3.3.17)

$$\underline{A}' = \underline{D} \cdot \underline{A} \cdot \underline{D}^{-1} = \begin{bmatrix} \underline{U} + \underline{W}\,\underline{\Omega} & 0 \\ 0 & \underline{\Omega}\,\underline{U}\,\underline{\Omega} - \underline{\Omega}\,\underline{W} \end{bmatrix}$$

It remains to investigate the effect of the transformation on $\underline{H}(c)$:

First, we note that $\underline{H}$ can be written as the product of 2^{r-1} factors, see (3.3.1o),

$$\underline{H} = D_1(\exp(rc),1,1, \ldots ,1,1,\exp(-rc)) \cdot \qquad (3.3.18)$$
$$\cdot D_2(1,\exp((r-2)c),1, \ldots ,1,\exp(-(r-2)c),1) \cdot \ldots$$

that is, as a product of the diagonal matrices D_1 , D_2 , ... In the following we shall obtain the matrices:

$$\underline{H}'_1 = \underline{D} \cdot D_1 \cdot \underline{D}^{-1}$$

and:

$$\underline{H}'_2 = \underline{D} \cdot D_2 \cdot \underline{D}^{-1}$$

and this will give us an idea how $\underline{H}' = \underline{D} \cdot \underline{H} \cdot \underline{D}^{-1}$ looks.

By direct computation, we find that:

$$\underline{H}'_1 = \begin{bmatrix} \cosh(rc) & 0 & \cdots & 0 & -\sinh(rc) \\ 0 & 1 & \cdots & 0 & 0 \\ \vdots & & & & \vdots \\ 0 & 0 & \cdots & 1 & 0 \\ -\sinh(rc) & 0 & \cdots & 0 & \cosh(rc) \end{bmatrix} \qquad (3.3.19)$$

and for the second factor:

$$\underline{H}'_2 = \begin{bmatrix} 1 & 0 & \cdots & 0 & 0 \\ 0 & \cosh((r-2)c) & \cdots & -\sinh((r-2)c) & 0 \\ \vdots & & & & \\ 0 & -\sinh((r-2)c) & \cdots & \cosh((r-2)c) & 0 \\ 0 & 0 & \cdots & 0 & 1 \end{bmatrix}$$

So that $\underline{H}' = \underline{H}'_1 \cdot \underline{H}'_2 \cdot \cdots$ is a product of Lorentz matrices corresponding to a first frame moving with uniform velocity $v_1 = C \tanh(rc)$ along x_1, then a second frame moving with $v_2 = C \tanh((r-2)c)$ along x_2, but having a different time abscissa, t_2, and so on ...

Here again, C is the velocity of light. We reiterate our previous statement, that we wish not to speculate, at this time, on the physical significance of this interpretation.

It is seen by inspection that: $\underline{H}'(0) = \underline{H}(0) = I_{(2^r \times 2^r)}$

and in this case the eigenvalue problem is reduced to the computation of the characteristic polynomial of two $2^{r-1} \times 2^{r-1}$ submatrices, see also item (3.3.17). In § 2 of this chapter, we took advantage of this situation when calculating the eigenvalues for the case when $c = 0$.

On inspecting (3.3.1o) , we see that: $\mathrm{Det}(\underline{R}) = \mathrm{Det}(\underline{H}).\mathrm{Det}(\underline{A}) = \mathrm{Det}(\underline{A})$,

and therefore: $\prod_{k=1}^{2^r} \lambda_k = f(a_1, \ldots, a_r)$, so that the product of the eigenvalues is independent of the scalar value of the external field. Therefore, a necessary and sufficient condition that at least one eigenvalue be zero is that $\mathrm{Det}(\underline{R})$ vanishes.

On considering values for c such that: $1 >> \delta > c > 0$, we can approximate, to any degree of accuracy, the eigenvalues of $\underline{R}' = \underline{D} \cdot \underline{R} \cdot \underline{D}^{-1}$ to those of $\underline{R}''$, where:

$$\underline{R}'' = D_1(\cosh(rc), 1, \ldots, 1, \cosh(rc)) \cdot D_2(1, \cosh((r-2)c), \ldots, \cosh((r-2)c), 1) \ldots \circ \underline{A}'(a_1, \ldots, a_r)$$

That is, we neglected the off-diagonal elements in the $\underline{H}_j'$, see (3.3.19) , which are sinh 's and can be made arbitrarily small by taking a sufficiently small c , and we retained the principal diagonal elements only. Therefore, the eigenvalues of $\underline{R}''$ are functions of: $\cosh(rc), \cosh((r-2)c), \ldots, a_1, \ldots, a_r$ and, for the greatest eigenvalue Λ , of $\underline{R}''$, which can be made arbitrarily close to the greatest eigenvalue of $\underline{R}'$, we have:

$$\Lambda = \Lambda(\cosh(rc), \cosh((r-2)c), \ldots, a_1, \ldots, a_r) \qquad (3.3.2o)$$

and accordingly:

$$\frac{\partial \Lambda}{\partial c} = \left[\frac{\partial \Lambda}{\partial(\cosh(rc))}\right] \cdot r \sinh(rc) + \left[\frac{\partial \Lambda}{\partial(\cosh((r-2)c))}\right] \cdot (r-2)\sinh((r-2)c) \qquad (3.3.21)$$

$$+ \ldots\ldots$$

Provided that the partial derivatives $\left[\frac{\partial \Delta}{\partial(\cosh(rc))}\right]$, $\left[\frac{\partial \Delta}{\partial(\cosh((r-2)c)}\right]$, ...

remain analytic as $c \longrightarrow 0$, and in view of the fact that:

$$\lim_{c \longrightarrow 0} \Lambda = \lambda_m \text{ , where } \lambda_m \text{ is the greatest eigenvalue}$$

of $\underline{R}'$, and furthermore in view of the possibility of showing that:

$$\lim_{c \longrightarrow 0} \left[\lambda_i' - \zeta_i'\right] = 0$$

(using a procedure similar to the one used in § 2 of this chapter)

where ζ_i are the eigenvalues of $\underline{R}''$, and finally in view of:

$$\prod_{i=1}^{2^r} \lambda_i = f(a_1, \ldots, a_r)$$

whose zeros do not depend on c , we are in a position to state the

CONJECTURE (3.3.22): If λ_m is the largest eigenvalue of $\underline{R}'$,

then:

$$\lim_{c \longrightarrow 0} \frac{\lambda_m'}{\lambda_m} = 0$$

where primes denote differentiation with respect to c . On using a convergence argument similar to the one used in § 2 of this chapter, we have the plausible conjecture:

CONJECTURE (3.3.23): The magnetisation of an Ising ring with arbitrary, but finite order of interactions is zero in the absence of an external magnetic field.

Our conjecture is fully supported by the theorem of VAN HOVE as stated, for example in (V) , § 4.11 .

§ 4) The straight line version of the linear model with simplified long range potential.Exact statistics.Ferromagnetism.

We consider the straight line model with all spins interacting.The interaction potential is generally a function of the distance separating the sites and here the distance between the j-th and k-th site is $|k - j|$. We denote the interaction potential between the k-th and the j-th site by:

$$u_i = u(|k - j|) \quad , \text{where} \quad |k - j| = i \qquad (3.4.1)$$

The Hamiltonian can be written as:

$$H(\underline{S}) = -h \sum_{k=1}^{N} S_k - \sum_{i=1}^{N-1} u_i \sum_{\substack{k>j \\ k-j=i}} S_k S_j \qquad (3.4.2)$$

and on setting: $\beta h = c$, $\beta u_i = a_i$, we have the reduced energy:

$$-\beta H(\underline{S}) = c \sum_{k=1}^{N} S_k + \sum_{i=1}^{N-1} a_i \sum_{\substack{k>j \\ k-j=i}} S_k S_j \qquad (3.4.2a)$$

It is seen by inspection that:

$$\left[\frac{\partial\ (-\beta H(\underline{S}))}{\partial c}\right]^2 = N + 2 \sum_{\substack{i \neq j \\ i>j}} S_i S_j$$

$$= N + 2 \sum_{i=1}^{N-1} \sum_{\substack{k>j \\ k-j=i}} S_k S_j \qquad (3.4.3)$$

$$= N + 2 \sum_{i=1}^{N-1} \frac{\partial(-\beta H(\underline{S}))}{\partial a_i} .$$

On using (3.4.3) , we have for the Boltzmann factor:

$$\frac{\partial 2}{\partial c^2}\,(\exp(-\beta H(\underline{S}))) \;=\; N\exp(-\beta H(\underline{S})) \;+\; 2\sum_{i=1}^{N-1}\frac{\partial}{\partial a_i}(\exp(-\beta H(\underline{S})))$$

Define as Ω_n the subset of (N) :

$$\Omega_n \;=\; \left\{\underline{S}\in(N) \;:\; \sum_{k=1}^{N} S_k \;=\; N-2n\right\}$$

and consider the sum:

$$G_n \;=\; \sum_{\underline{S}\in\Omega_n}\exp(-\beta H(\underline{S})) \qquad (3.4.4)$$

Then we have:

$$\frac{\partial^2 G_n}{\partial c^2} \;=\; N\,G_n \;+\; 2\sum_{i=1}^{N-1}\frac{\partial G_n}{\partial a_i} \qquad (3.4.5)$$

Let us set:

$$G_n \;=\; \exp\left[\,-\frac{N}{2(N-1)}\sum_{i=1}^{N-1}a_i\,\right]\,R_n(c,a_1,\ \cdots\ ,a_{N-1}) \qquad (3.4.6)$$

And then we have:

$$\frac{\partial^2 R_n}{\partial c^2} \;=\; 2\sum_{i=1}^{N-1}\frac{\partial R_n}{\partial a_i} \qquad (3.4.7)$$

The most general closed form solution for this is:

$$R_n\,(c,a_1,\ \cdots\ ,a_{N-1}) = \text{constant}\cdot\exp\Big(\,bc+\frac{1}{2}\sum_{i=1}^{N-1}p_i a_i\Big) \qquad (3.4.8)$$

The most general solution R_n as in (3.4.8) is accompanied by the condition:

$$b^2 = \sum_{i=1}^{N-1} p_i$$

and if we set:

$$p_i = \frac{b^2 r_i}{\sum_i r_i} \qquad (3.4.9)$$

where the r_i are positive constants to be determined, then the condition is satisfied and we can write:

$$R_n(c,a_1, \dots) = A \exp\left(bc + \frac{b^2}{2}\left[\frac{\sum r_i a_i}{\sum r_i}\right] \right) \qquad (3.4.10)$$

Now R_n must satisfy the first boundary condition:

$$R_n(c,0, \dots ,0) = G_n(c,0, \dots ,0).$$

so that:

$$A \exp(bc) = \binom{N}{n} \exp((N - 2n)c) \qquad (3.4.10a)$$

and this determines A and b. The sum in the exponential can reasonably be called the <u>weighted mean</u> of the reduced interaction potentials a_i, and we denote it by:

$$M(\underline{a}) = \left[\frac{\sum r_i a_i}{\sum r_i}\right] , \quad \underline{a} = (a_1, \dots ,a_{N-1}) \qquad (3.4.11)$$

It is seen to be a linear functional on the "interaction vector" $\underline{a}$.
The weighted mean was derived for the sum over the subset Ω_n of (N) .
Since $0 \leq n \leq N$, we insert the additional argument n and call:

$M(n , \underline{a})$ the weighted mean at n .

In view of (3.4.6) , (3.4.10) and the boundary condition (3.4.10a) , and for a sufficiently large N , we have the partition function as a sum of N+1 terms:

$$Q_N = \exp\Big(- \frac{1}{2} \sum_{i=1}^{N-1} a_i \Big) \quad \sum_{n=0}^{N} \binom{N}{n} \exp\Big((N-2n)c + \frac{(N-2n)^2}{2} M(n,\underline{a})\Big) \qquad (3.4.12)$$

We propose to investigate a model with a long range interaction potential of the form:

$$-u_i = - \frac{\eta}{N} \quad , \text{ for } i = 1,2, \ldots , N-1$$

and η is a constant. For reasons of convenience, we define: $\beta u_i = \frac{\beta \eta}{N} = 2a$.

Accordingly, (3.4.12) takes the form:

$$Q_N = \exp(- aN) \cdot \sum_{n=0}^{N} \binom{N}{n} \exp\Big((N-2n)c + \frac{(N-2n)^2}{2} \cdot 2a\Big) \qquad (3.4.13)$$

since the constant interaction potential remains unchanged on taking the means at n .

Thus for very large N there is only a weak, residual interaction between the spins ; but as the mathematics will show, this residual interaction is still sufficient to produce the pronounced cooperative phenomenon of spontaneous magnetisation. Since the interaction potential is independent of the distance separating the spins the model must be considered as somewhat "unphysical" , but so are models with first or second (or any finite) order of interaction, and therefore we can say that the model of § 2 of this chapter, and the present one, lie on opposite ends of the spectrum of simplifications. It is for this reason that we compare them in mathematical detail. Furthermore, we should like to point out that the result will be mathematically equivalent to the BRAGG - WILLIAMS solution as presented in (I). However, we build on a different premise and our result obtains with mathematical rigour.

We proceed to obtain the closed form solution of the limit:

$$\lim_{N \to \infty} \left[Q_N \right]^{\frac{1}{N}} = \exp(-\beta f)$$

From (3.4.13) and for large but finite N :

$$Q_N = \exp(-\frac{\beta \eta}{2}) \sum_{n=0}^{N} \binom{N}{n} \exp((N-2n)c + (N-2n)^2 a) \qquad (3.4.14)$$

The closed form of this sum exists as an operator formulation, as we shall show in chapter IV.

For any real p we have the identity:

$$\sqrt{\frac{a}{\pi}} \int_{-\infty}^{+\infty} \exp(-a(x^2 - 2px)) \, dx = \exp(a p^2)$$

which is a linear operation on exp(2apx) . Consequently, we have for Q_N :

$$Q_N = \sqrt{\frac{a}{\pi}} \exp(-\frac{\beta \eta}{2}) \int_{-\infty}^{+\infty} \exp(-ax^2) \sum_{n=0}^{N} \binom{N}{n} \exp((N-2n)(c + 2ax))dx$$

On carrying out the summation over n we obtain:

$$Q_N = \sqrt{\frac{a}{\pi}} \exp(-\frac{\beta \eta}{2}) 2^N \int_{-\infty}^{+\infty} \exp(-ax^2) \cosh^N(c + 2ax)dx \qquad (3.4.15)$$

Let us define:

$$I_N = \int_{-\infty}^{+\infty} \exp(-ax^2) \cosh^N(c + 2ax) \, dx \qquad (3.4.16)$$

Then we have for the limit:

$$\lim_{N \to \infty} \frac{1}{N} \ln Q_N = \lim_{N \to \infty} \frac{1}{N} \left[\frac{1}{2} \ln \frac{a}{\pi} + N \ln 2 - \frac{\beta \eta}{2} + \ln I_N \right]$$

$$= \ln 2 + \lim_{N \to \infty} \frac{1}{N} \ln I_N$$

Thus we are led to consider the limit: $\lim_{N \to \infty} \left[I_N \right]^{\frac{1}{N}}$

We return to:

$$I_N = \int_{-\infty}^{+\infty} \exp(-ax^2) \cosh^N(c + 2ax) \, dx \qquad (3.4.16)$$

where : $a = \frac{\beta \eta}{2N}$. We do a change of variable : $x = N u$,

and so:

$$I_N = N \int_{-\infty}^{+\infty} \exp(-\frac{b u^2}{2} N) \cosh^N (c + bu) \, du \qquad (3.4.16a)$$

where: $b = \beta \eta$. Consider now the function $f(u)$ given by:

$$f(u) = \exp(-\frac{b u^2}{2}) \cosh(c + bu) \qquad (3.4.17)$$

This function is continuous and therefore measurable .The following is quoted from (IV),page 91 : If (r,s) is an infinite interval of the real line and if $f(u)$ is measureable and essentially bounded,then:

$$\lim_{N \to \infty} \left[\int_r^s |f(u)|^N \, du \right]^{\frac{1}{N}} = \lim_{n \to \infty} \lim_{N \to \infty} \left[\int_{E_n} |f(u)|^N \, du \right]^{\frac{1}{N}} \qquad (3.4.18)$$

$$= \sup^{o} |f(u)|$$

where E_n is a sequence of finite intervals such that: $E_1 \subset E_2 \subset \cdots$, each E_n lies in (r,s) , and $\bigcup_n E_n = (r,s)$.

We return to $f(u) = \exp(-\frac{b\,u^2}{2})\cosh(c + bu)$, and observe that:

i) $f(u) = |f(u)| \geq 0$, on the real line ,

ii) $\lim_{u \to \pm\infty} f(u) = 0$. Furthermore, $f(u)$ is bounded above by the greatest of its maxima.

We determine the extrema of $f(u)$ by the condition $f'(u) = 0$, and this leads to the equation:

$$u = \tanh(c + bu) \qquad (3.4.19)$$

Let u_1 determine the greatest of the maxima of $f(u)$, then:

$$f(u_1) = \sup^{o} |f(u)| \qquad (3.4.20)$$

Next we choose the sequence of nested intervals $E_n = (-n , +n)$, for $n = 1,2, \cdots$, and it follows that $\bigcup_n E_n = R$, the real line .

From (3.4.18) and the foregoing follows that the limit exists,and :

$$\lim_{N \to \infty} \left[I_N \right]^{\frac{1}{N}} = \sup^{o} f(u) \qquad (3.4.21)$$

Furthermore,the limit is uniformly attained as this follows from the proof given in our reference.Consequently,we have the reduced partition function:

$$q = \lim_{N \to \infty} \frac{1}{N} \ln Q_N = \ln 2 + \ln(\sup^{o} f(u)) \qquad (3.4.22)$$

That is: $$q(c,b) = \ln 2 - \frac{b u_1^2}{2} + \ln(\cosh(c + bu_1)) \qquad (3.4.22a)$$

where u_1 determines the essential supremum and is a solution of (3.4.19).

The magnetisation, as seen from above, is :

$$\lim_{c \to 0} \frac{\partial q}{\partial c} = \tanh(bu_1) = u_1 \qquad (3.4.23)$$

where in view of (3.4.19): $$u_1 = \tanh(bu_1) \qquad (3.4.19a)$$

We must admit that the formal proof of uniform convergence on a finite interval of 1/T of:

$$\frac{\partial}{\partial c} (\frac{1}{N} \ln Q_N)$$, as shown in § 2 of this

chapter, is lacking here. On the other hand we always have for the magnetisation per spin and spin moment that:

$$| m_N(c,T) | \leq 1 \quad , \qquad \text{for all } N ,$$

and so the sequence remains, at least, bounded. And while there may possibly be oscillations for a finite subsequence of N 's , we would expect, on physical grounds, that the "tail" of the sequence converges uniformly, for as the assembly reaches macroscopic size the addition of one more spin would not disturb the physical behaviour of the entire assembly to any detectable extend.

Thus the magnetisation is the real value u_1 , such that $f(u_1) = \sup^{o} f(u)$.

The accompanying requirements are:

$$f'(u_1) = 0 \quad , \quad f''(u_1) < 0 \quad , \quad f(u) \leq f(u_1) \qquad (3.4.24)$$

We shall confine ourselves to positive values of u , or possibly zero. (negative values correspond to $c \to 0^-$)

Let us rewrite (3.4.19a) by setting $u = \frac{w}{b}$ .Then we have to solve:

$$m(0,T) = \frac{w}{b} = \tanh w \qquad (3.4.25)$$

The intersection of the curves $g(w) = \frac{w}{b}$ and $h(w) = \tanh w$ is shown in figure I , and a projective plot of the magnetisation too. It is seen that for $b < 1$ there is just one solution for (3.4.25), that is $w = 0$, whereas for $b > 1$, there are two intersections, namely $w = 0$ and $w = w^{\circ}$.

We show that for $b<1$, $u_1 = 0$ is a maximum . We already have $f'(0) = 0$, and we show that for $b < 1$, $f'(u) < 0$, and since no further root obtains , $f'(u)$ will not change sign and therefore $f(u)$ decreases.

Now: $f'(u) = b \exp(-\frac{b u^2}{2})(\sinh(bu) - u \cosh(bu))$, and (3.4.25) consider the infinitesimal $\delta u > 0$, then we have for $b < 1$,

$$b^{-1} f'(\delta u) \doteq \delta u(b - 1) < 0 \qquad \text{QED.}$$

On the other hand,for $b > 1$, we also have $f'(0) = 0$, but the same argument as above shows that:

$$b^{-1} f'(\delta u) \doteq \delta u(b - 1) > 0$$

and no further change of sign occurs until $u_1 > 0$. Therefore, $f(u)$ increases up to u_1 and $f(u_1) = \sup^{\circ} f(u)$. QED.

Thus the critical temperature,the CURIE point,is given by $b = \frac{\mathcal{M}}{k T} = 1$

If we define the CURIE temperature by $T_o = \frac{n}{k}$, then the magnetisation is given by:

$$m(0,T) = 0 \qquad \text{for} \quad T > T_o$$

$$m(0,T) > 0 \qquad \text{for} \quad T < T_o \qquad (3.4.26)$$

Again,we refer the reader to our projective plot.

We have shown,by concrete example,that long range interaction,although simplified,causes the cooperative phenomenon of spontaneous magnetisation in the one dimensional model.By contrast,the model of § 2 of this chapter exhibits no such behaviour.Our results agree with the theorem of VAN HOVE, an improved version of which is given in (V) , § 4.11 .

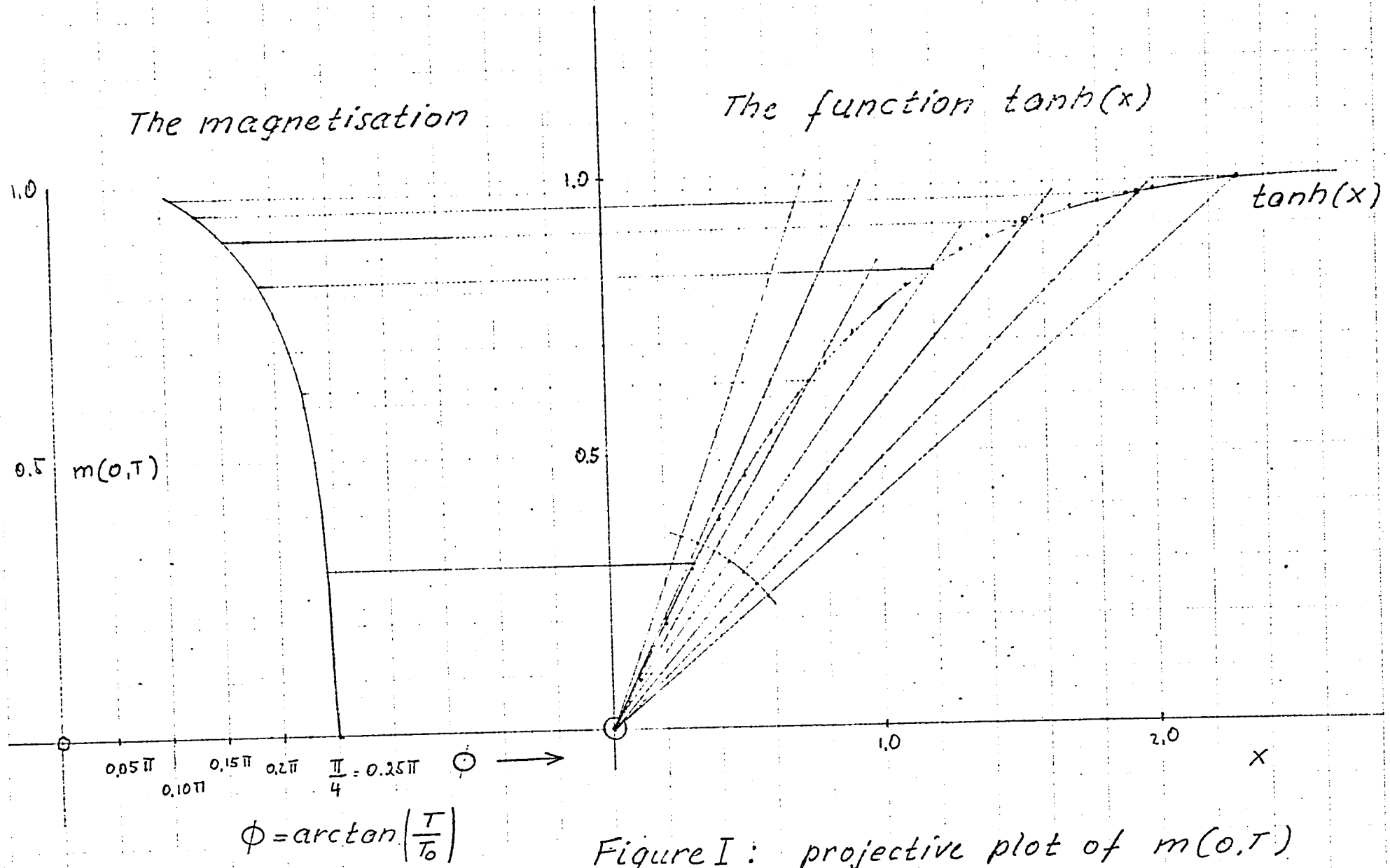
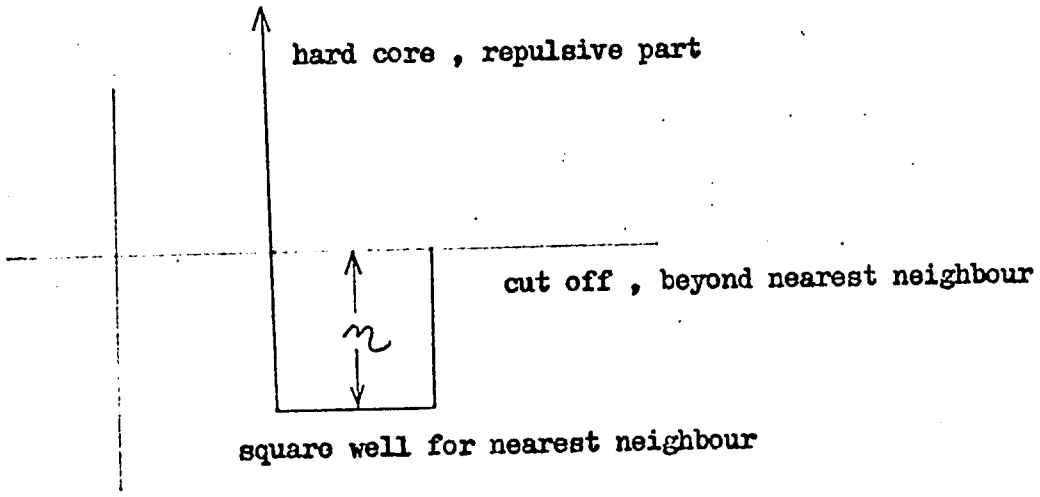


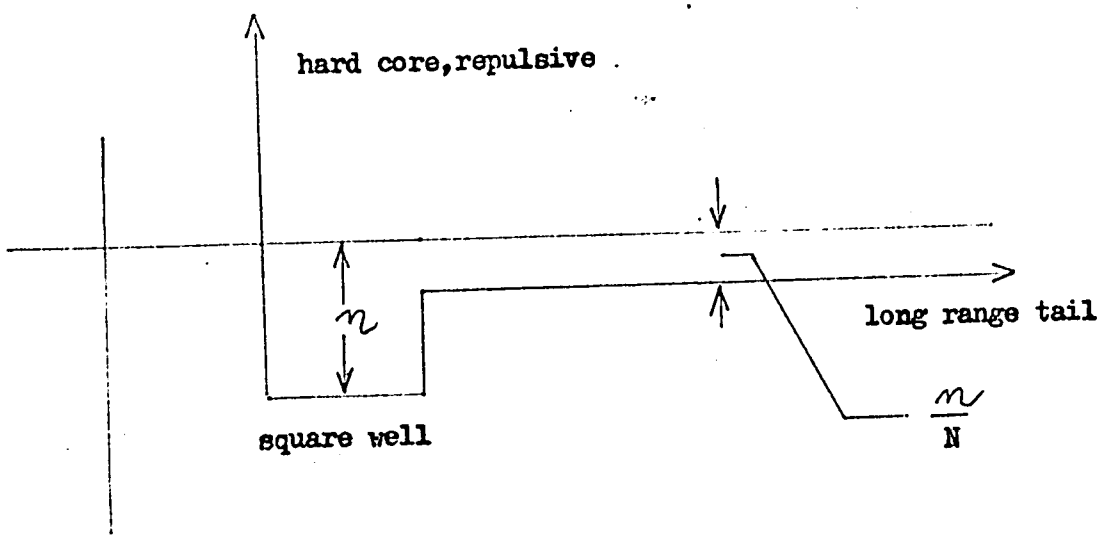
Figure I : projective plot of $m(0,T)$

§ 5 The linear lattice fluid with long range interaction potential.

Let us return to the model discussed in § 1 of this chapter. There, we tacitly used a potential of the form:



Now we propose to investigate a one dimensional assembly having a realistic first order potential plus a long range "tail" .



Let us set: $c = \phi + u$, $\beta\eta = a$, $-\beta\mu = u$, as in § 1 , (3.2)

Let $\underline{S} \in (N)$. Then the reduced energy has the form:

$$-\beta H(\underline{S}) = c \sum_{k=1}^{N} S_k + a \sum_{k=2}^{N} S_k S_{k-1} + \frac{a}{N} \sum_{\substack{k>j \\ k-j>1}} S_k S_j \qquad (3.5.1)$$

We have the identity: $$\sum_{\substack{k>j \\ k-j>1}} S_k S_j = \frac{1}{2}(n^2 - n) - \sum_{k=2}^{N} S_k S_{k-1}$$

where : $n = \underline{S} \cdot \underline{S}$. On the other hand , $n = \sum_{k=1}^{N} S_k$, and therefore:

$$-\beta H(\underline{S}) = n(c - \frac{a}{2N}) + (a - \frac{a}{N}) \sum_{k=2}^{N} S_k S_{k-1} + \frac{an^2}{2N}$$

and for sufficiently large N :

$$-\beta H(\underline{S}) \doteq n c + \frac{an^2}{2N} + a \sum_{k=2}^{N} S_k S_{k-1} \qquad (3.5.2)$$

Accordingly, we adopt as starting point the reduced Hamiltonian:

$$-\beta H(\underline{S}) = \frac{an^2}{2N} + c \sum_{k=1}^{N} S_k + a \sum_{k=2}^{N} S_k S_{k-1} \qquad (3.5.3)$$

On using the identity:

$$\sqrt{\frac{a}{2N\pi}} \int_{-\infty}^{+\infty} \exp(- \frac{a}{2N} (x^2 - 2nx))dx = \exp(\frac{an^2}{2N}) \qquad (3.5.4)$$

we have:

$$Z_N = \sqrt{\frac{a}{2N\pi}} \int_{-\infty}^{+\infty} \exp(- \frac{ax^2}{2N}) \sum_{\underline{S} \in (N)} \exp((c + \frac{ax}{N}) \sum_{k=1}^{N} S_k + a \sum_{k=2}^{N} S_k S_{k-1}) dx$$

where we denoted by Z_N the partition function. The indicated sum is:

$$Q_N ((c + \frac{ax}{N}) , a) \quad , \qquad \text{see } (3.1.12)$$

Hence:

$$Z_N = \sqrt{\frac{a}{2N\pi}} \int_{-\infty}^{+\infty} \exp\left(-\frac{ax^2}{2N}\right) \; Q_N\left(\left(c+\frac{ax}{N}\right), a\right) dx \qquad (3.5.5)$$

Let us change variables: $x = Nu$, then :

$$Z_N = \sqrt{\frac{aN}{2\pi}} \int_{-\infty}^{+\infty} \exp\left(-\frac{au^2}{2} N\right) Q_N((c+au), a) \, du \qquad (3.5.6)$$

We confine our attention to the integral:

$$I_N = \int_{-\infty}^{+\infty} \exp\left(-\frac{au^2}{2} N\right) Q_N((c+au), a) \, du \qquad (3.5.7)$$

and seek to evaluate the limit:

$$\lim_{N \to \infty} \left[I_N\right]^{\frac{1}{N}} \qquad (3.5.7a)$$

From: (3.1.12) $Q_N = A p_1^N + B p_2^N$, and we equate Q_N to G_N^N :

$$G_N^N = A p_1^N + B p_2^N \qquad (3.5.8)$$

that is:

$$G_N = p_1 \left[A + B r^N\right]^{\frac{1}{N}} \quad , \quad r = \frac{p_2}{p_1}$$

It is seen that : $\lim_{N \to \infty} G_N = p_1$, since $r < 1$

Furthermore, since $p_1 , p_2 > 0$, and $Q_N > 0$, always have that $A + B r^N > 0$, for all N Next we use the initial conditions on N :

$$(Q_o =) \quad 1 = A + B$$

$$(Q_1 =) \quad \exp(c) + 1 = A p_1 + B p_2 \qquad (3.5.9)$$

An explicit calculation would show that: $A , B > 0$, and it follows that : $A + B r^N < 1$, and so we have the inequalities :

$$I_N \leq \int_{-\infty}^{+\infty} \exp(- \frac{au^2}{2} N) p_1^N \, du \qquad (3.5.10)$$

and:

$$\int_{-\infty}^{+\infty} \exp(- \frac{au^2}{2} N) A p_1^N \, du \leq I_N$$

It can now be shown that:

$$\lim_{N \to \infty} \left[I_N \right]^{\frac{1}{N}} = \lim_{N \to \infty} \left\{ \int_{-\infty}^{+\infty} \exp(- \frac{au^2}{2} N) p_1^N \, du \right\}^{\frac{1}{N}}$$

$$= \sup^o (\exp(- \frac{au^2}{2}) p_1) \qquad (3.5.11)$$

Here we used essentially the same reasoning as in § 4 of this chapter. It is noted that the function $A((c+au) , a)$ has no poles on the real line.

Let $f(u) = \exp\left(-\frac{au^2}{2}\right) p_1((c + au) , a)$, where we take p_1 from (3.10) of § 1 of this chapter. We must have: $f(u_1) = \sup^{\circ} f(u)$, and this is accompanied by the conditions:

$$f'(u_1) = 0 \quad , \quad f''(u_1) < 0 \quad , \quad f(u) \leqq f(u_1)$$

the first of which leads to the equation:

$$u = \frac{1}{2}\left\{ 1 + \frac{\sinh\left(\frac{1}{2}(c + a + au)\right)}{\sqrt{\sinh^2\left(\frac{1}{2}(c + a + au)\right) + \exp(-a)}} \right\} \qquad (3.5.12)$$

Let us recall that: $a = \frac{n}{kT}$, $c = -\frac{\mu}{kT} + \frac{1}{2} \ln\left[\frac{2\pi mkT}{[\hbar^2]^{\circ}}\right]$

where $[\hbar^2]^{\circ}$ is to say that we only use the physical dimension of $\hbar^2$.

We rewrite (3.5.12) as: (set $2w = au$)

$$w\left(\frac{2kT}{n}\right) = \frac{1}{2}\left\{ 1 + \frac{\sinh(g(T) + w)}{\sqrt{\sinh^2(g(T) + w) + \exp\left(-\frac{n}{kT}\right)}} \right\} \qquad (3.5.13)$$

where $g(T) = \frac{n - \mu}{2kT} + \frac{1}{4} \ln\left[\frac{2\pi mkT}{[\hbar^2]^{\circ}}\right]$ (3.5.14)

From § 2 of chapter II , we have the density per particle and particle mass given as:

$$\rho(n, \mu, T) = \frac{\partial}{\partial c}\left(\lim_{N \to \infty} \frac{1}{N} \ln Z_N \right) \qquad (3.5.15)$$

On the other hand: $$q = \lim_{N \to \infty} \frac{1}{N} \ln Z_N$$

$$= \ln \sup^{o} f(u) \qquad (3.5.16)$$

$$= -\frac{a u_1^2}{2} + \ln p_1((c + a u_1), a)$$

and so:

$$\rho(\eta, \mu, T) = \frac{p_1'}{p_1}$$, where the prime denotes differentiation with respect to c . Then it is seen by inspection that:

$$\rho(\eta, \mu, T) = u_1 = w_1\left[\frac{2kT}{\eta}\right] \qquad (3.5.17)$$

see (3.5.12) and (3.5.13), and u_1 is that root which determines $\sup^{o} f(u)$.

We define two parametric families of curves:

$$h(w,T) = \frac{1}{2}\left\{1 + \frac{\sinh(g(T) + w)}{\sqrt{\sinh^2(g(T) + w) + \exp(-\frac{\eta}{kT})}}\right\} \qquad (3.5.18)$$

and:

$$l(w,T) = w\left[\frac{2kT}{\eta}\right]$$

which is a parametric pencil of straight lines emanating from the origin.

In what follows we shall confine our discussion to the standard chemical state which, by definition has unit fugacity and therefore $\mu = 0$. See, for example (V), page 205 . This simplifies our task by eliminating one constant. The function g(T) reduces to:

$$g(T) = \frac{\eta}{2kT} + \frac{1}{4} \ln\left[\frac{2\pi mkT}{[h^2]^{o}}\right] \qquad (3.5.19)$$

Now consider the points of intersection of $h(w,T)$ and $l(w,T)$ with $y = \frac{1}{2}$ whose abscissae are given by:

$$w_h = -g(T) = -\frac{\eta}{2kT} - \frac{1}{4}\ln\left[\frac{2\pi mkT}{[\hbar^2]^\circ}\right] \qquad (3.5.20)$$

and:

$$w_l = \frac{\eta}{4kT}$$

Denote by dots differentiation with respect to <u>decreasing</u> T, ($T \downarrow$), then the <u>velocities</u> towards the right, as $T \downarrow$ are given by :

$$\dot{w}_h = \frac{1}{4T} - \frac{\eta}{2kT^2}$$

and : for $T \downarrow$ (3.5.21)

$$\dot{w}_l = \frac{\eta}{4kT^2}$$

so that for sufficiently low T : $\dot{w}_l > \dot{w}_h$ and w_l, if initially to the left of w_h, eventually "overtakes" w_h. This takes place as:

$$w_h = w_l$$

that is:

$$\frac{3\eta}{4kT} + \frac{1}{4}\ln\left[\frac{2\pi mkT}{[\hbar^2]^\circ}\right] = 0 \qquad (3.5.22)$$

which is rewritten as:

$$\zeta\left[\frac{6\pi\eta m}{[\hbar^2]^\circ}\right] = \ln[\zeta] \qquad (3.5.23)$$

where : $$\zeta = \frac{1}{kT}\left[\frac{[\hbar^2]^\circ}{2\pi m}\right]$$

The left side of (3.5.23) has a non-negative slope and therefore a necessary condition for a root ζ to exist is that:

$$\zeta \geq 1 \quad , \quad \text{and so:} \qquad T \leq \left[\frac{\hbar^2}{2\pi mk}\right]^{\circ} \sim \frac{10^{16}}{m}$$

which, on physical grounds is a realistic upper bound on T . On taking g(T) from (3.5.19) and comparing with (3.5.22) , we see that for , say $T = 10^5$, we have $g(T) << 0$, whereas $1(w,T)$ virtually coincides with the y-axis. For such a temperature T :

$$h(0,T) \cong \frac{1}{2}\left[1 + \tanh(g(T)) \right] = 0^+$$

and this corresponds to zero density. Moreover, the abscissa w_h lies initially at the right of w_1 . The analytic behaviour of $\rho(\eta, 0, T)$ is now determined by the intersection of $h(w,T)$ and $1(w,T)$ as T decreases. Thus the density curve will be determined by the modes of intersection of two "floating curves" . Eventually, the point of intersection $w_o = w_1 = w_h$, see (3.5.2o), will occur. We investigate the possible modes of intersection locally at w_o .

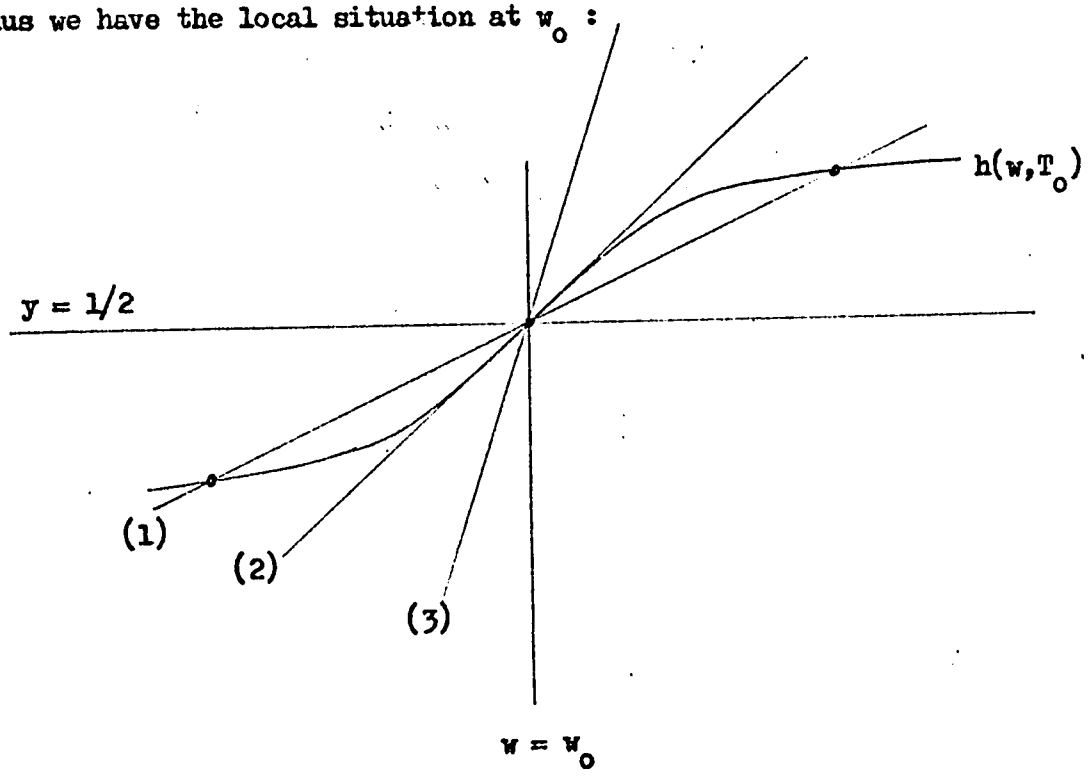
From (3.5.18) we deduce that for:

$$\begin{aligned} &\text{i)} \quad w < w_o \quad , \quad h(w,T_o) < \frac{1}{2} \\ &\text{ii)} \quad w = w_o \quad , \quad h(w,T_o) = \frac{1}{2} \\ &\text{iii)} \quad w > w_o \quad , \quad h(w,T_o) > \frac{1}{2} \end{aligned} \qquad (3.5.24)$$

where T_o is the solution for equation (3.5.22).

As discussed before, the two curves meet at w_o , and clearly : $h(w_o,T_o) = 1(w_o,T_o)$

Thus we have the local situation at w_o :



The crucial question is whether:

$$\begin{aligned} &(1): && \frac{2kT_o}{\eta} && < && h'(w_o,T_o) \\ &(2): && \frac{2kT_o}{\eta} && = && h'(w_o,T_o) \\ &(3): && \frac{2kT_o}{\eta} && > && h'(w_o,T_o) \end{aligned} \qquad (3.5.25)$$

where primes denote differentiation with respect to w . Let us recall (3.5.22):

$$\frac{n}{kT_o} = -\frac{1}{3} \ln \left[\frac{2\pi mkT}{[h^2]^o} \right] \qquad (3.5.22)$$

and we calculate $h'(w_o,T_o)$: (note that $w_o + g(T_o) = 0$)

$$h'(w_o,T_o) = \frac{1}{2}\left[\frac{2mkT\pi}{[h^2]^o} \right]^{-\frac{1}{6}} \qquad (3.5.26)$$

From (3.5.22) we see that necessarily: $\left[\frac{2\pi mkT}{[\hbar^2]^\circ}\right]_o < 1$,

and therefore: $h'(w_o, T_o) > \frac{1}{2}$, and this condition is not explicitly depending on T_o or η , rather it is a condition for the solvability of (3.5.22) for non-negative T_o . Therefore (1) is implied by :

$$\frac{2kT}{\eta}_o < \frac{1}{2}$$, and similarly, (2) and (3)

imply that:

$$\frac{2kT}{\eta}_o > \frac{1}{2} \qquad (3.5.27)$$

We rewrite (3.5.22) to:

$$2kT_o = \left[\frac{[\hbar^2]^\circ}{\pi m}\right] \exp\left(-\frac{3\eta}{kT_o}\right) \qquad (3.5.22a)$$

and the condition (2) of (3.5.25) can be written as:

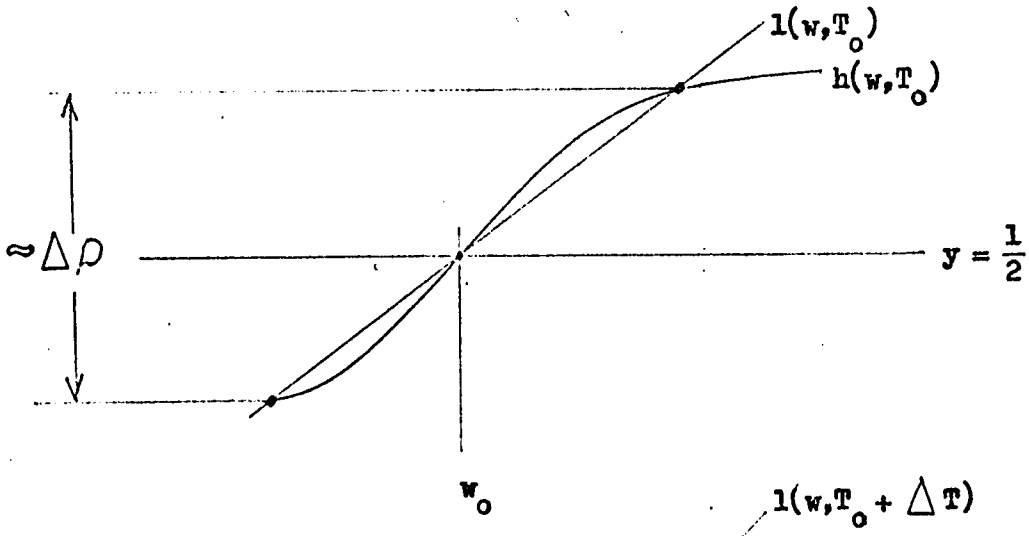
$$2kT_o = \eta \exp\left(\frac{\eta}{kT_o}\right) \qquad (3.5.25a)$$

On dividing (3.5.22a) by (3.5.25a) , we obtain:

$$1 = \left[\frac{[\hbar^2]^\circ}{\pi m \eta}\right] \exp\left(-\frac{4\eta}{kT_o}\right) \qquad (3.5.28)$$

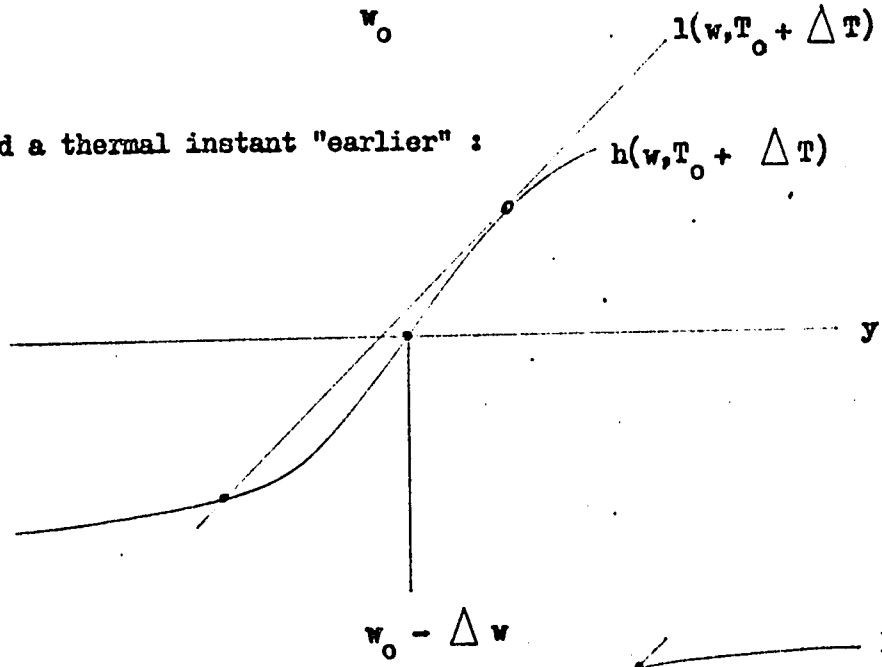
Therefore, both conditions , (1) and (3) of (3.5.25) can be obtained by a suitable change of (possibly both) η or m . The possibility of equality as in (2) of (3.5.25) is not excluded by (3.5.22) in any a priori fashion, whether (2) is excluded and one of the remaining two possibilities occurs depends on η and m . We note that the numerical values of η and m are small.

We shall first discuss the implication of (1) of (3.5.25) . Let us therefore assume that (1) occurs.Then at (w_o, T_o) we have the situation:



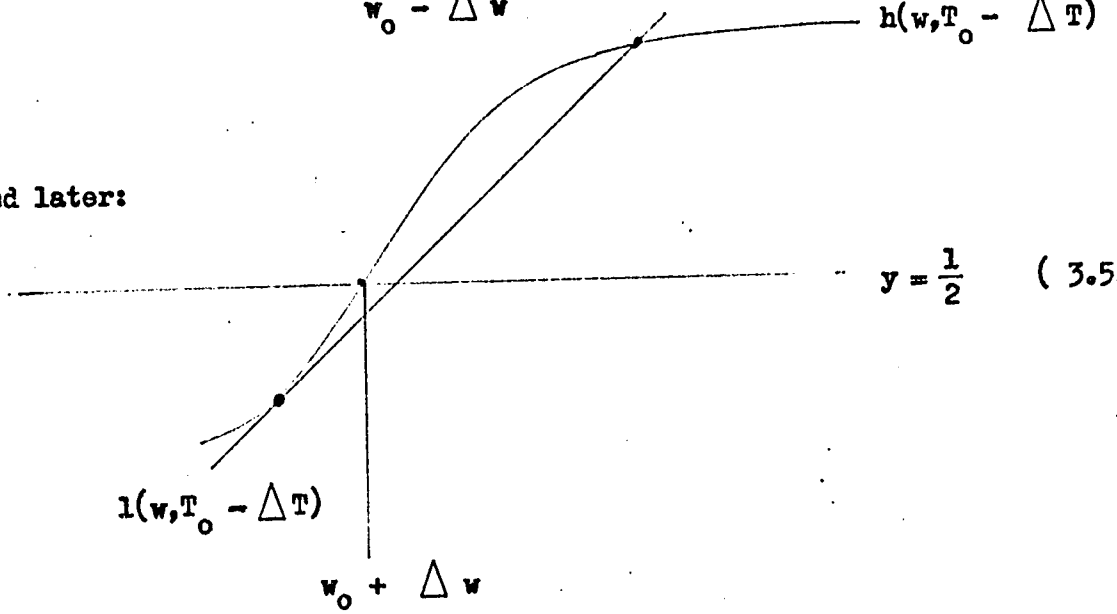
(3.5.29a)

and a thermal instant "earlier" :



(3.5.29b)

and later:



(3.5.29c)

The three situations,(3.5.29a) to (3.5.29c) describe a change of phase ! We justify this claim as follows:as T decreases we eventually reach (3.5.29b) and the point of intersection with the upper branch occurs.As T decreases further,the lower point of intersection abruptly ceases to exist and the remaining point of intersection,on the upper branch,moves continuously to the right as T decreases further,and correspondingly,the density increases. Then we imagine the same process in reverse motion,that is starting from a lower temperature T and increasing T up to beyond $T_o + \Delta T$.

Then we have two mutually exclusive possibilities:either the lower branch point of intersection determines $\sup^o f(u)$ as long as it exists ; or else the upper branch point of intersection acts in this way.But as soon as one of the two points ceases to exist,the remaining one determines the $\sup^o f(u)$. This follows from:

$$f(u) \geq 0 \quad \text{and} \quad \lim_{u \to \pm\infty} f(u) = 0$$

and there can only be one maximum but no minimum for finite u .

We refer the reader to figure II.There,for definiteness,we assume that the upper branch point of intersection determines,as soon as it occurs, the $\sup^o f(u)$.The ordinate values of the points of intersection are projected to the left onto a density scale and the so obtained density plot exhibits the shape of a classical phase change.The density,as a function of T,is discontinuous at a critical temperature T_c which is close to T_o , as previously discussed,and may be estimated from (3.5.22) . The rate of change of the density is seen to increase beyond any bound at T_c , for at T_c^+ we have $\sup^o f(u) = f(u_I)$, where u_I is determined by the lower branch point of intersection.At T_c^- we have $\sup^o f(u) = f(u_{II})$ and u_{II} is determined by the upper branch point of intersection.The sudden "jump" in ρ , $\Delta\rho$ is of the magnitude as shown in (3.5.29a) and gives the difference of the densities corresponding to phase(II) and phase(I).

Therefore, for decreasing T , the rate of change of the density is given by:

$$\left[\frac{\partial \rho}{\partial T}\right]_{T_o} = -\left[\frac{\rho(T_c^+) - \rho(T_c^-)}{T_c^+ - T_c^-}\right] \doteq \lim_{\Delta T \to 0} \frac{\Delta u}{\Delta T}$$

where: $\Delta u = u_{II} - u_I > 0$. Hence the rate of change diverges to ∞ at T_c . The analytic behaviour of the density $\rho(\eta, 0, T)$, as well as the qualitative shape of its graph, agrees with the general theory of phase change as discussed by YANG and LEE in (VI) . The mathematical "mechanism" of the phase change is apparently not determined by a zero in the grand canonical partition function, as suggested by Yang and Lee, but rather by the mode of intersection of two "floating" curves. This observation applies, of course, only to our model with its particular potential.

It remains to discuss the case (3) of (3.5.25) . Here only one point of intersection exists at all temperatures T. The density increases very slowly as the point moves to the right on the lower branch until it reaches the proximity of T_o . Then there is a rapid, but continuous increase of $\rho(\eta, 0, T)$ as the point moves over the S-shaped part of the curve, thereafter the increase is only minimal and the density approaches asymptotically to unity.

We wish to estimate the rate of change of the density at T_o . At T_o we have $h'(w_o, T_o) > \frac{1}{2}$, and so:

$$\left[\frac{\partial \rho}{\partial T}\right]_{T_o} \doteq h'(w_o, T_o)\, \Delta \dot{w}_{l,h}$$

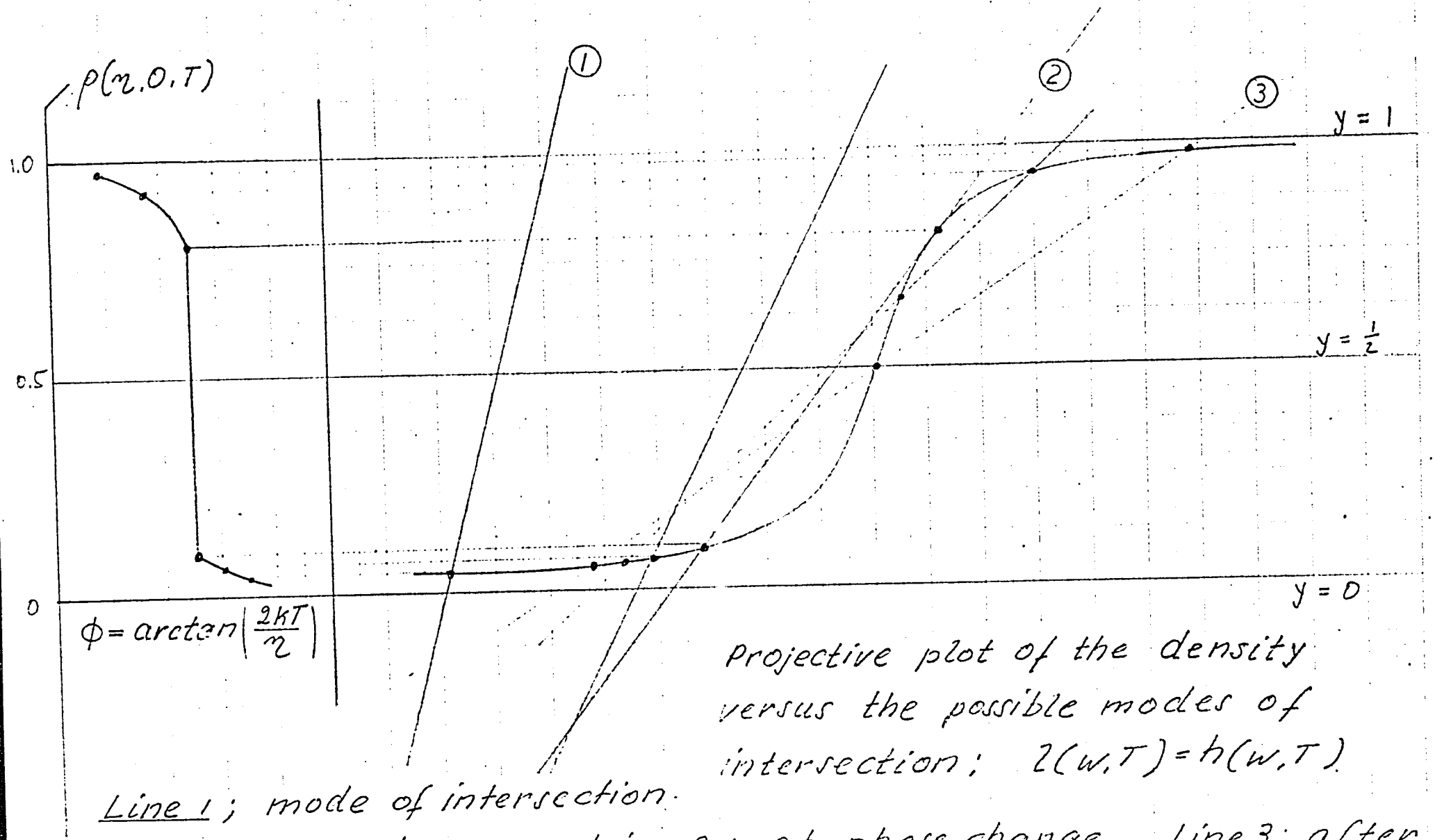
where $\Delta \dot{w}_{l,h} = \dot{w}_l - \dot{w}_h$, see (3.5.21) .

Therefore:

$$\left[\frac{\partial \rho}{\partial T}\right]_{T_o} > \frac{1}{2}\left[\frac{3}{4kT_o^2} - \frac{1}{4T_o}\right] \qquad (3.5.30)$$

Again,as opposed to the one in § 1 of this chapter,our present model, its one-dimensionality notwithstanding,can have a phase change and we have demonstrated by concrete example that this is caused by the long range part of the interaction potential.The same square well,but without the long range "tail" leads to a closed from partition function which is analytic in its arguments for physically acceptable values,in particular the density is a continuous function of T . By contrast,the present model,as case (1) of (3.5.25) occurs,has a discontinuous partition function,the critical point being near T_o which in principle can be calculated from (3.5.22). The critical temperature,in turn,is then a function of η and m . Accordingly,we have a corresponding discontinuity in the equation of state,in the internal energy (and hence the specific heat diverges at the critical temperature) and,as demonstrated,in the density.

Relative positions Figure II ; Mechanism of phase change.



projective plot of the density versus the possible modes of intersection; $l(w,T) = h(w,T)$.

Line 1; mode of intersection before phase change, Line 2: at phase change, Line 3: after

not drawn to scale

Chapter IV

Further propositions

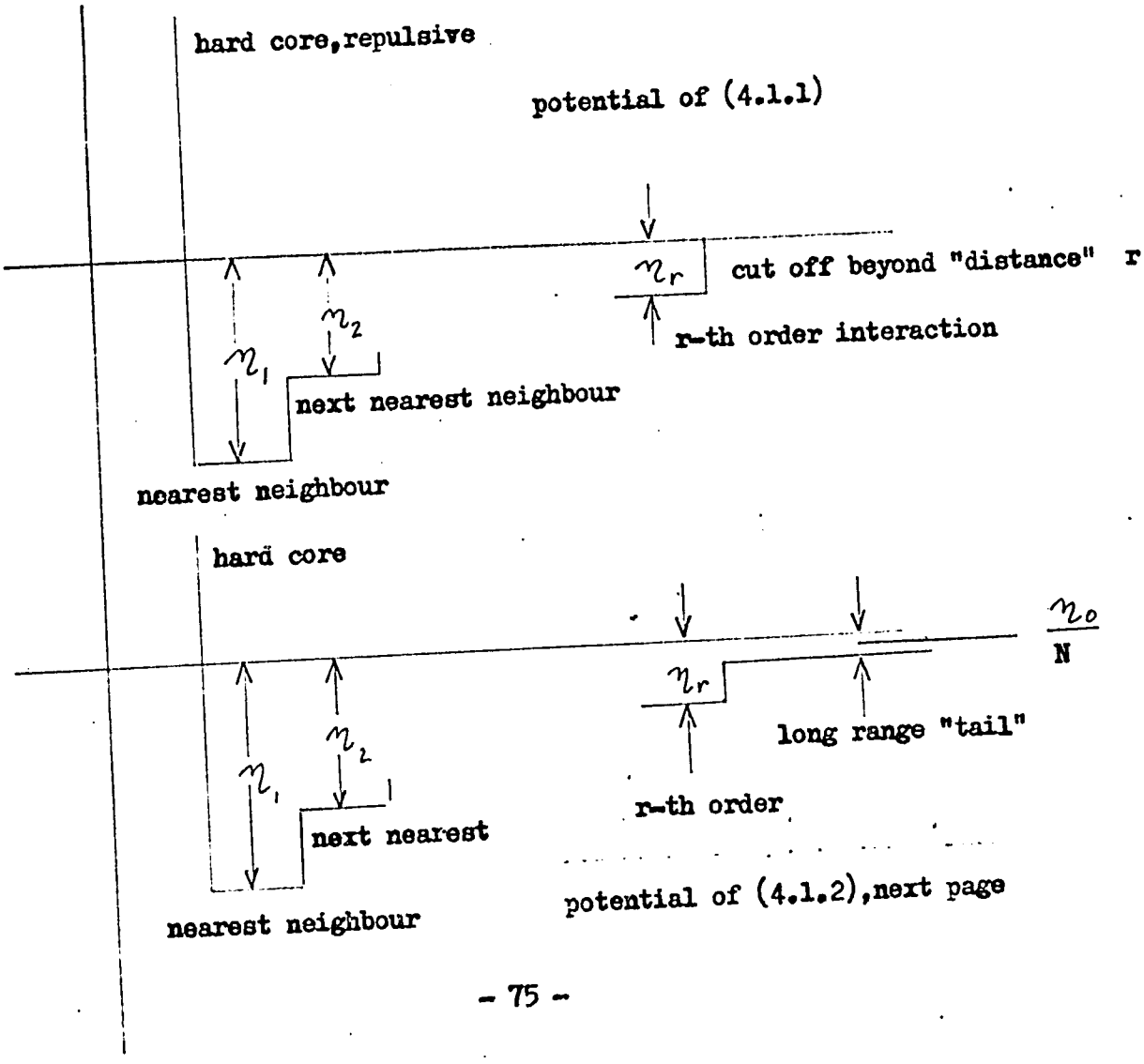
§ 1 The principle of combination of finite order interaction potentials with simplified long range interaction. Existence of closed form solutions.

We consider the straight line version of the one-dimensional model. Denote by $\eta_1, \eta_2, \dots, \eta_r$ the finite range interaction potentials up to and inclusive order r. The reduced Hamiltonian has the form:

$$-\beta H(\underline{S}) = c \sum_{k=1}^{N} S_k + a_1 \sum_{k=2}^{N} S_k S_{k-1} + \dots + a_r \sum_{k=r+1}^{N} S_k S_{k-r} \qquad (4.1.1)$$

where as usual: $\beta h = c$, $\beta \eta_i = a_i$, $i = 1,2, \dots, r$

and $\underline{S} \in (N)$. Accordingly, we have a potential of the form (schematically):



Then we take the reduced Hamiltonian of (4.1.1) and define $-\beta H_1(\underline{S})$ by:

$$-\beta H_1(\underline{S}) = -\beta H(\underline{S}) + \frac{a_o}{N} \sum_{\substack{j>k \\ j-k>r}} S_j S_k \qquad (4.1.2)$$

where the subscript 1 denotes "long range" , and $\beta \mathcal{M}_o = a_o$.

(See previous page). Let us note that:

$$2 \sum_{\substack{j>k \\ j-k>r}} S_j S_k = \left[\sum_{k=1}^{N} S_k \right]^2 - N - 2 \sum_{k=2}^{N} S_k S_{k-1} - \dots - 2 \sum_{k=r+1}^{N} S_k S_{k-r}$$

and therefore (4.1.2) can be written as:

$$-\beta H_1(\underline{S}) = \frac{a_o}{2N} \left[\sum_{k=1}^{N} S_k \right]^2 - \frac{a_o}{2} + c \sum_{k=1}^{N} S_k + \qquad (4.1.3)$$

$$+ \left[a_1 - \frac{a_o}{2N} \right] \sum_{k=2}^{N} S_k S_{k-1} + \dots + \left[a_r - \frac{a_o}{2N} \right] \sum_{k=r+1}^{N} S_k S_{k-r}$$

Therefore, for sufficiently large N we adopt as starting point the reduced Hamiltonian:

$$-\beta H_1(\underline{S}) = \frac{a_o}{2N} \left[\sum_{k=1}^{N} S_k \right]^2 - \frac{a_o}{2} + c \sum_{k=1}^{N} S_k + \qquad (4.1.4)$$

$$+ a_1 \sum_{k=2}^{N} S_k S_{k-1} + \dots + a_r \sum_{k=r+1}^{N} S_k S_{k-r}$$

We recall the identity:

$$\exp\left(\frac{a_o}{2} \frac{n^2}{N} \right) = \sqrt{\frac{a_o}{2N\pi}} \int_{-\infty}^{+\infty} \exp\left(- \frac{a_o}{2N} (x^2 - 2nx) \right) dx$$

On using this identity, we have for the Boltzmann factor with $-\beta H_1(\underline{S})$:

$$\exp(-\beta H_1(\underline{S})) = \exp(-\frac{a_o}{2}) \sqrt{\frac{a_o}{2N\pi}} \int_{-\infty}^{+\infty} \exp(-\frac{a_o x^2}{2N}) \quad \text{. continued} \qquad (4.1.5)$$

$$\text{continuation .} \quad \exp\left((c + \frac{a_o x}{N}) \sum_{k=1}^{N} S_k + a_1 \sum_{k=2}^{N} S_k S_{k-1} + \cdots + a_r \sum_{k=r+1}^{N} S_k S_{k-r} \right) dx$$

so that: (4.1.6)

$$Z_N = \sum_{\underline{S} \in (N)} \exp(-\beta H_1(\underline{S})) = \exp(-\frac{a}{2}o) \sqrt{\frac{a_o}{2N\pi}} \int_{-\infty}^{+\infty} \exp(-\frac{a}{2}o\frac{x}{N})^2 \; Q_N((c + \frac{a_o x}{N}), a_1, \ldots, a_r) dx$$

where: $Q_N(c, a_1, \cdots, a_r)$ is the closed from partition function for the straight line model with interactions up to and inclusive r .

On doing a change of variable: $x = Nu$, we obtain: (4.1.7)

$$Z_N = \exp(-\frac{a}{2}o) \sqrt{\frac{a_o N}{2\pi}} \int_{-\infty}^{+\infty} \exp(-\frac{a_o N x^2}{2}) \; Q_N((c + a_o x), a_1, \cdots, a_r) dx$$

If the partition function Q_N , for the straight line model with interactions up to and inclusive r , can be written as:

$$Q_N = A_1 p_1^N + A_2 p_2^N + \cdots$$

where $A_1, A_2, \cdots$ are analytic functions of c , on the real line , and $A_1, A_2, \cdots > 0$, $A_1 + A_2 + \cdots = 1$, and $p_1 \geq p_2, \cdots$

with $p_1, p_2, \ldots > 0$, then we have:

$$\int_{-\infty}^{+\infty} \exp\left(-\frac{a_o N x^2}{2}\right) A_1 p_1^N \, dx \leq \int_{-\infty}^{+\infty} \exp\left(-\frac{a_o N x^2}{2}\right) Q_N \, dx$$

$$\leq \int_{-\infty}^{+\infty} \exp\left(-\frac{a_o N x^2}{2}\right) p_1^N \, dx$$

and it can be shown that:

$$\lim_{N \to \infty} \left[Z_N \right]^{\frac{1}{N}} = \lim_{N \to \infty} \left\{ \int_{-\infty}^{+\infty} \exp\left(-\frac{a_o N x^2}{2}\right) p_1^N \, dx \right\}^{\frac{1}{N}} \qquad (4.1.8)$$

$$= \sup^o \left[\exp\left(-\frac{a_o x^2}{2}\right) p_1((c + a_o x), a_1, \ldots, a_r) \right]$$

We had demonstrated this approach, for the lattice fluid with first order interactions plus long range tail, in § 5 of chapter III.

Let x_o determine the $\sup^o$ in (4.1.8) . Then the equation of state is given by:

$$\frac{Pv}{kT} = -\frac{a_o x_o^2}{2} + \ln\left[p_1((c + a_o x_o), a_1, \ldots, a_r) \right]$$

The necessary condition that $f'(x_o) = 0$, leads to:

$-a_o x p_1 + a_o p_1' = 0$, or $x = \frac{p_1'}{p_1}$, and x_o is a root of this equation. Primes denote differentiation with respect to x .

On setting $a_o x = \left(\frac{\eta_o}{kT}\right) x = u$, we have : $u\left(\frac{kT}{\eta_o}\right) = \frac{p_1'}{p_1}$ (4.1.9)

Again, we are confronted with the problem of determining the intersection of the parametric pencil of straight lines emanating from the origin:

$$l(u,T) = \left| \frac{kT}{m_0} \right| u \qquad (4.1.10)$$

with the parametric family of curves:

$$h(u,T) = \left[\frac{p_1' \left[(c+u), a_1, \ldots, a_r \right]}{p_1 \left[(c+u), a_1, \ldots, a_r \right]} \right] \qquad (4.1.11)$$

and the modes of intersection determine the thermodynamic behaviour of the model. In § 4 of chapter III , we had demonstrated the method for the straight line version of the linear model having initially "zero order" interactions and we saw that spontaneous magnetisation occurs in the absence of an external magnetic field. The next improvement, in this line of thinking, is to consider a first order square well plus long range "tail" . Now the partition function for the straight line version having first order interactions only, in the presence of an external field, is given in terms of the recurrence relation of LEFF and FLICKER (which will be discussed in more detail in § 3):

$$Q_{N+1} = 2 \exp(a)\cosh(c)\, Q_N - 2 \sinh(2a)\, Q_{N-1} \qquad (4.1.12)$$

and the general solution to (4.1.12) is given by:

$$Q_N = A\, p_1^N + B\, p_2^N \qquad (4.1.12a)$$

where:

$$p_{1,2} = \exp(a)\left[\cosh(c) \pm \sqrt{\sinh^2(c) + \exp(-4a)} \right] \qquad (4.1.13)$$

The function $A(c,a)$ is non-negative and has no poles on the real line. The root p_1 is seen to be the greatest.

Using the fact that $A > 0$, (this follows from $Q_N > 0$, which in turn implies that $A + B\, r^N > 0$, for all N , and $r = \frac{p_2}{p_1} < 1$) , and following our general procedure,one can show that:

$$\lim_{N \to \infty} \left[Z_N \right]^{\frac{1}{N}} =$$

$$= \lim_{N \to \infty} \left\{ \int_{-\infty}^{+\infty} \exp\left(-\frac{ax^2}{2} \right) p_1((c + ax) , a)^N \, dx \right\}^{\frac{1}{N}}$$

$$= \sup^{o} f(x) \quad , \quad \text{here } Z_N \text{ is the partition function}$$

for the long range interaction model and $f(x)$ is given in terms of p_1 , $f(x) = \exp\left(-\frac{ax^2}{2} \right) p_1((c + ax) , a)$, where p_1 is taken from (4.1.13).

The value x_o such that $f(x_o) = \sup^{o} f(x)$, is a root of the equation:

$$x = \left[\frac{p_1'((c + ax) , a)}{p_1 ((c + ax) , a)} \right] \qquad (4.1.14)$$

where primes denote differentiation with respect to x . On making the substitution : $ax = u$, and differentiating $p_1((c + ax) , a)$, see (4.1.13) we obtain the equation:

$$u \left(\frac{kT}{\eta} \right) = \frac{\sinh(c + u)}{\sqrt{\sinh^2(c + u) + \exp(-4a)}} \qquad (4.1.15)$$

Following essentially the same line of reasoning as in § 4 of Chapter III, (see also items (3.4.22),(3.4.22a) and (3.4.23)),we obtain for the magnetisation:

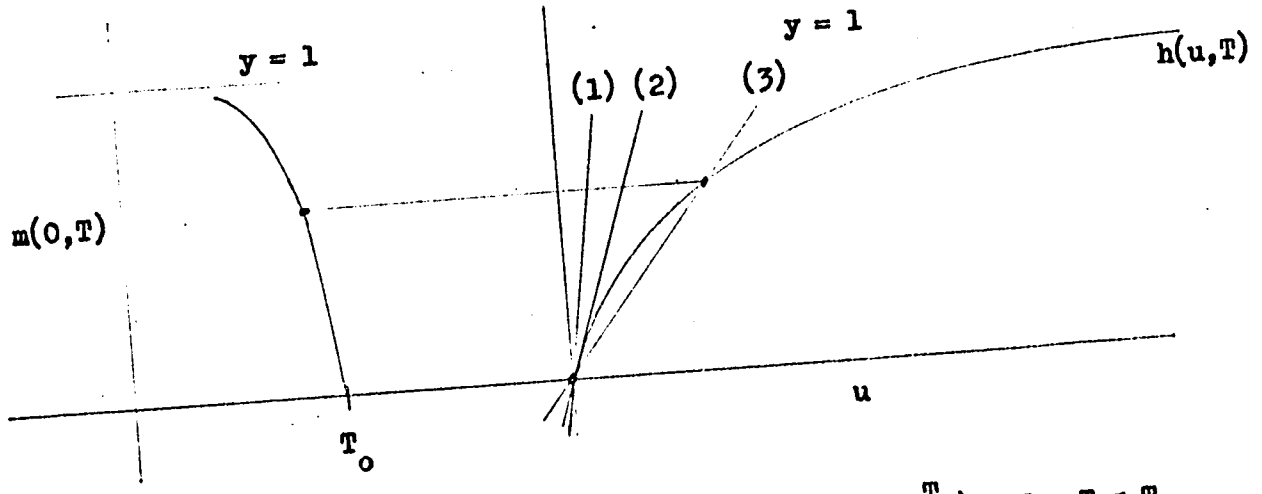
$$m\,(0,T) = u \left(\frac{kT}{\eta} \right) = h(u,T) \qquad (4.1.15a)$$

Here again, the magnetisation is determined by the modes of intersection of two parametric curves. The function:

$$h(u,T) = \frac{\sinh(u)}{\sqrt{\sinh^2(u) + \exp(-4a)}} \qquad (4.1.16)$$

may be described as a distorted $\tanh(u)$ and it is convex-up on R^+.

The value $x = 0 = u$ always satisfies the equation $u\left(\frac{kT}{\eta}\right) = h(u,T)$ and, accordingly, as long as it is the sole root of (4.1.15), the magnetisation $m(0,T) = 0$. As the temperature decreases there will eventually be a second root for (4.1.15), and an argument similar to the one in § 4 of Chapter III (see item (3.4.26)) would show that the second point of intersection, as soon as it occurs, determines the $\sup^o f(x)$. The two situations are shown below:



The left side is a projective plot: $m(0,T)$ vs. $\arctan\left(\frac{T}{T_o}\right)$, for $T < T_o$, and $m(0,T) = 0$, for $T > T_o$. This corresponds in spirit to our result in § 4 of chapter III. There is, however, a significant difference. We shall show that the Curie point is raised by a factor more than doubling the critical temperature of <u>this</u> model as compared with the one in § 4 in chapter III.

A moment of reflection will show that the second point of intersection emerges and begins to move up on $h(u,T)$ as soon as the temperatur T_o, given as the root of :

$$\frac{kT}{\mu}_o = h'(0,T_o) \qquad (4.1.17)$$

is reached and below T_o. This amounts to solving:

$\frac{kT}{\mu}_o = \exp(\frac{2\mu}{kT_o})$, which is equivalent to: $w = \exp(\frac{2}{w})$,

and $w \cong 2.35$ is the root. Accordingly : $T_o = 2.35 \frac{\mu}{k}$,

and for $T > T_o$, $m(0,T) = 0$, for $T < T_o$, $m(0,T) > 0$.

We have shown that the model with realistic first order interactions plus long range "tail" has a higher critical temperature, in fact raised by a factor of 2.35 as compared with the model in § 4 of chapter III . One may say that this potential gives more stability to the magnetic structure of the assembly, it endures a higher temperature before the ordered state of the spins is destroyed.

§ 2 The operator formulation of the Ising model

We begin our presentation by considering the one dimensional model, regardless whether ring model or straight line version. We start from first principles.

Let: $$\underline{S} \in \{+1,-1\}^N = (N)$$

The most general form of the Hamiltonian is given by:

$$H(\underline{S}) = -h \sum_{k=1}^{N} S_k - \sum_{j>k} v(j,k) S_j S_k \qquad (4.2.1)$$

and $v(j,k)$ is the interaction potential between the j-th and the k-th site, depending only on the "distance" $|j-k|$, and therefore: $v(j,k) = v(k,j)$.

Consider now the function:

$$\psi(\underline{S},\underline{X}) = \exp\left(\sum_{k=1}^{N} S_k X_k \right) = \exp(\underline{S} \cdot \underline{X}) \qquad (4.2.2)$$

where $\underline{X}$ is an N-dimensional vector whose components are real variables.

We define: $$D_{jk} = \partial_j \partial_k \quad , \text{ for } j \neq k \text{ , and } \partial_i = \frac{\partial}{\partial X_i} = D_i$$

Then it is seen that the operators commute:

$$\text{for } j \neq k \text{ , } i \neq l \text{ , } \quad \left[D_{jk} , D_{il} \right] = 0 \text{ , } \quad \left[D_k , D_{ij} \right] = 0 \qquad (4.2.3)$$

and obviously: $$\left[D_j , D_k \right] = 0$$

The commutation rules are stated with respect to the function $\psi(\underline{S},\underline{X})$ as defined by (4.22).

Furthermore, we have:

$$v(j,k)\, D_{jk}\, \psi(\underline{S},\underline{X}) = v(j,k)\, S_j S_k\, \psi(\underline{S},\underline{X})$$

and similarly: (4.2.4)

$$h\, D_k\, \psi(\underline{S},\underline{X}) = h\, S_k\, \psi(\underline{S},\underline{X})$$

so that $\psi(\underline{S},\underline{X})$ is an eigenfunction of the operator family:

$$\left\{ D_k \, , \, D_{jk} \right\} \quad , \quad j \neq k \, , \quad j,k = 1,2, \ldots ,N \qquad (4.2.5)$$

We are now in a position to define a Hamiltonian o p e r a t o r :

$$\underline{H}_{op} = -h \sum_{k=1}^{N} D_k - \sum_{j>k} v(j,k)\, D_{jk} \qquad (4.2.6)$$

and it is seen that: $\underline{H}_{op}\, \psi(\underline{S},\underline{X}) = H(\underline{S})\, \psi(\underline{S},\underline{X})$ (4.2.7)

Because of our commutation rules (4.2.3) we are in a position to write:

$$\exp(-\beta\, \underline{H}_{op})\, \psi(\underline{S},\underline{X}) = \exp(-\beta H(\underline{S}))\, \psi(\underline{S},\underline{X}) \qquad (4.2.8)$$

Furthermore: $\psi(\underline{S},\underline{0}) = 1$, where: $\underline{0} = (0, \ldots ,0)$

and also:

$$\sum_{\underline{S} \in (N)} \psi(\underline{S},\underline{X}) = 2^N \prod_{k=1}^{N} \cosh(X_k) \qquad (4.2.9)$$

It is therefore seen that: (4.2.10)

$$Q_N = \sum_{\underline{S} \in (N)} \exp(-\beta H(\underline{S})) = 2^N \exp(-\beta\, \underline{H}_{op}) \prod_{k=1}^{N} \cosh(X_k) \Bigg\}_{\underline{X} = \underline{0}}$$

Equation (4.2.10) is the operator formulation of the one dimensional model. It applies equally well to the ring model or to the straight line version, for our derivation was independent of the enumeration scheme. On replacing the integers j and k by 2 or 3-dimensional vectors whose components are integers, we easily extend the operator formulation to 2 or 3 dimensions.

We can alter our approach somewhat by defining:

$$\underline{U}_{op} = \sum_{j>k} v(j,k)\, D_{jk} \qquad (4.2.11)$$

Upon a moment 's reflection, we see that:

$$\exp(-\beta \underline{U}_{op})\ \psi(\underline{S},\underline{X})\Big\}_{\underline{X}=\underline{h}} = \exp(-\beta H(\underline{S}))$$

, please do see remark I at the end of this section !

where: $\underline{h} = (h, \ldots, h)$. Consequently, we obtain:

$$Q_N = \exp(-\beta \underline{U}_{op}) \sum_{\underline{S} \in (N)} \psi(\underline{S},\underline{X})\Big\}_{\underline{X}=\underline{h}} \qquad (4.2.12)$$

or:

$$Q_N = 2^N \exp(-\beta \underline{U}_{op}) \prod_{k=1}^{N} \cosh(X_k)\Big\}_{\underline{X}=\underline{h}}$$

Let us briefly return to (3.4.14) of § 4 of chapter III. There we had:

$$Q_N = \exp(-\frac{\beta m}{2}) \sum_{n=0}^{N} \binom{N}{n} \exp((N-2n)c + (N-2n)^2 a) \qquad (3.4.14)$$

It is readily deduced that: $\exp(a \frac{\partial^2}{\partial c^2}) \exp(pc) = \exp(pc + ap^2)$

Therefore, the promised operator formulation of the partition function is:

$$Q_N = \exp(-\frac{\beta n}{2})\exp(a\frac{\partial 2}{\partial c^2}) \sum_{n=o}^{N} \binom{N}{n} \exp((N-2n)c)$$

so that:

$$Q_N = \exp(-\frac{\beta n}{2}(1 - \frac{1}{N} \frac{\partial^2}{\partial c^2})) 2^N \cosh^N (c) \qquad (4.2.13)$$

on recalling that: $a = \frac{\beta n}{2N}$, and the square of the differential operator commutes with the exponential of a constant.

The operator principle is easily applied to the lattice fluid. On retaining our standard notation:

$$c = -\beta\mu + \phi \quad , \quad \{0,1\}^N = (N) \qquad (4.2.14)$$

and for interaction potentials $u(j,k)$ between the j-th and k-th cell, we have the Hamiltonian: (reduced form)

$$-\beta H(\underline{S}) = c \sum_{k=1}^{N} S_k + \sum_{j>k} a(j,k) S_j S_k$$

where $a(j,k) = -\beta v(j,k)$, and the corresponding operator is:

$$-\beta \underline{H}_{op} = c \sum_{k=1}^{N} D_k + \sum_{j>k} a(j,k) D_{jk} \qquad (4.2.15)$$

Again we have: $(\underline{S},0) = 1$, but now the sum is somewhat different:

$$\sum_{\underline{S} \in (N)} \psi(\underline{S},\underline{X}) = \prod_{k=1}^{N} (\exp(X_k) + 1) \qquad (4.2.16)$$

The sum (4.2.16) can as well be written as:

$$\sum_{\underline{S} \in (N)} \psi(\underline{S},\underline{X}) = 2^N \prod_{k=1}^{N} \exp\left(\frac{1}{2} X_k\right) \cosh\left(\frac{1}{2} X_k\right) \qquad (4.2.16a)$$

Accordingly, the closed form operator formulation is:

$$Q_N = 2^N \exp\left(-\beta \underline{H}_{op}\right) \prod_{k=1}^{N} \exp\left(\frac{1}{2} X_k\right) \cosh\left(\frac{1}{2} X_k\right) \Bigg\}_{\underline{X} = \underline{0}} \qquad (4.2.17)$$

Again, extension to higher dimensions is possible, see our remarks preceding item (4.2.11) .

In the following section, we shall demonstrate a concrete example of an application of this operator formalism to the straight line version of the linear Ising model.

(Remark I: We beg the readers indulgence ! Unlike our previous convention, here h corresponds to βh , so that on doing actual calculations one has to substitute $h \longrightarrow \beta h$. However, for the remaining part of this chapter, we shall not deviate from this deviation.)

§ 3 The recurrence relation of LEFF and FLICKER.

We apply the operator formulation to obtain a recurrence relation for the partition functions of the straight line version of the linear Ising model. The model has first order interaction only and the magnetic field is present. This recurrence relation was first derived and published in a paper by Leff and Flicker , (VIII) , but their mode of derivation is a bit lenghty.

We use the formulation (4.2.12) . In view of the first order interaction, we set:

$$\text{for } j \neq k \ , \quad v(j,k) = 0 \ , \ \text{if} \ \ |j-k| > 1 \qquad (4.3.1)$$

and :

$$v(j,j-1) = -\eta \quad j = 2,3, \ldots ,N$$

furthermore, as usual: $\eta\beta = a$

Accordingly, we have:

$$Q_N = 2^N \exp\Big(a \sum_{j=2}^{N} D_{jj-1} \Big) \prod_{k=1}^{N} \cosh(X_k) \Big\}_{\underline{X} = \underline{h}} \qquad (4.3.2)$$

we commute $\exp(a\, D_{NN-1})$ with the product up to N-2 and consider:

$$\exp(a\, D_{NN-1}) \cosh(X_{N-1})\cosh(X_N) = \qquad (4.3.3)$$

$$= \cosh(a)\cosh(X_N)\cosh(X_{N-1}) + \sinh(a)\sinh(X_N)\sinh(X_{N-1})$$

We observe that the operator family contains no further operator acting on X_N , therefore we set $X_N = h$ and obtain:

$$= \exp(a)\cosh(h)\cosh(X_{N-1}) - \sinh(a)\cosh(h - X_{N-1}) \qquad (4.3.3a)$$

having done a minor rearrangement.

Then it is seen that:

$$Q_N = 2\exp(a)\cosh(h)\ \ 2^{N-1}\exp\Big(a\sum_{j=2}^{N-1} D_{jj-1}\Big)\ \prod_{k=1}^{N-1}\cosh(X_k)\Big\}_{\underline{X}'=\underline{h}'}$$

$$- 2\sinh(a)\ \ 2^{N-1}\exp\Big(a\sum_{j=2}^{N-1} D_{jj-1}\Big)\ \prod_{k=1}^{N-2}\cosh(X_k)\cosh(h - X_{N-1})\Big\}_{\underline{X}'=\underline{h}'} \qquad (4.3.4)$$

where $\underline{X}'$ and $\underline{h}'$ are the N-1 dimensional editions of $\underline{X}$ and $\underline{h}$, respectively.

One notes that the first term of the right side of (4.3.4) is:

$$2\exp(a)\cosh(h)\ Q_{N-1}$$

We proceed with the second term of the right side of (4.3.4). There, we commute $\exp(a\, D_{N-1\ N-2})$ with the product up to N-3 and consider:

$$\exp(a\, D_{N-1\ N-2})\cosh(X_{N-2})\cosh(h - X_{N-1}) \qquad (4.3.5)$$

and this is seen to equal: $\cosh(a\, D_{N-2})\cosh(X_{N-2})$, on setting $X_{N-1} = h$, for the family is now exhausted with respect to X_{N-1}. (The reader will note that $\cosh(a\, D_{N-2})$ is well defined). A moment of reflection shows that:

$$2\cosh(a\, D_{N-2})\cosh(X_{N-2}) =$$

$$= \cosh(X_{N-2} + a) + \cosh(X_{N-2} - a) = 2\cosh(a)\cosh(X_{N-2})$$

Therefore, the second term in the sum (4.3.4) is equal to :

$$- 4\sinh(a)\cosh(a)\ \ 2^{N-2}\exp\Big(a\sum_{j=2}^{N-2} D_{jj-1}\Big)\ \prod_{k=1}^{N-2}\cosh(X_k)\Big\}_{\underline{X}''=\underline{h}''} \qquad (4.3.6)$$

In (4.3.6) , $\underline{X}^{\prime\prime}$ denotes the N-2 dimensional edition of $\underline{X}$, and similarly for $\underline{h}^{\prime\prime}$. It is seen by inspection that (4.3.6) is equal to:

$$- 4 \sinh(a)\cosh(a)\, Q_{N-2}$$

and we have shown that:

$$Q_N = 2 \exp(a)\cosh(h)\, Q_{N-1} - 2 \sinh(2a)\, Q_{N-2} \qquad (4.3.7)$$

and this is the recurrence relation of Leff and Flicker. The general solution for (4.3.7) has the form:

$$Q_N = A\, p_1^N + B\, p_2^N$$

where $p_{1,2}$ are the roots of the characteristic polynomial of (4.3.7) , and the constants A and B can be determined from:

$$\begin{aligned} (\, Q_0 = \,) \quad & 1 = A + B \\ (\, Q_1 = \,) \quad & 2\cosh(h) = A\, p_1 + B\, p_2 \end{aligned} \qquad (4.3.8)$$

Leff and Flicker discussed to some extend the case where : $p_1 = p_2$. This condition has no bearing on the result ! From the theory of recurrence relations (IX), we have for this case:

$$Q_N = p_1^N (A + N B) \,, \qquad (4.3.9)$$

and therefore:

$$\lim_{N \to \infty} \frac{1}{N} \ln Q_N = p_1 + \lim_{N \to \infty} \frac{1}{N} \ln (A + N B)$$

$$= p_1$$

The recurrence relation (4.3.7) allows us to calculate the closed form solution of the partition function $Q_N(h,a)$. Let us, symbolically, create a "slot" for the reduced second order interaction potential a_2 . We would write:

$$Q_N(h,a_1,a_2) \quad \text{of which} \quad Q_N(h,a_1,0) \quad \text{is the special case}$$

of first order interactions only, just discussed. In concluding this section, we shall present the rather curious:

EXCHANGE LEMMA: If $Q_N(h,a_1,a_2)$ is the closed form solution of the partition function for the straight line version of the linear Ising model with up to and inclusive second order interactions plus spin to field interaction, then this function exhibits the peculiar property:

$$Q_N(0,x,y) = 2\, Q_{N-1}(x,y,0) \qquad (4.3.10)$$

for any two real variables x and y .

Proof: Let us write $Q_N(0,x,y)$ as the sum:

$$Q_N(0,x,y) = \sum_{\underline{S} \in (N)} \exp(-\beta H(\underline{S})) \qquad (4.3.11)$$

where:

$$-\beta H(\underline{S}) = x \sum_{j=2}^{N} S_j S_{j-1} + y \sum_{j=3}^{N} S_j S_{j-2} \qquad (4.3.11a)$$

On the other hand:

$$Q_{N-1}(x,y,0) = \sum_{\underline{S}' \in (N-1)} \exp(-\beta H'(\underline{S}')) \qquad (4.3.12)$$

where $\underline{S}'$ is the N-1 dimensional edition of $\underline{S}$, and:

$$-\beta H'(\underline{S}') = x \sum_{j=1}^{N-1} S_j' + y \sum_{j=2}^{N-1} S_j' S_{j-1}' \qquad (4.3.12a)$$

Let $\underline{S} \in (N)$. It is easy to see that: $S_j S_{j-2} = (S_j S_{j-1})(S_{j-1} S_{j-2})$ for $j = 3,4, \ldots ,N$. Next we define:

$$S'_{j-1} = S_j S_{j-1} \quad , \quad j = 2,3, \ldots ,N \qquad (4.3.13)$$

And then we define a correspondence by:

$$\phi : (N) \longrightarrow (N-1) \qquad (4.3.14)$$

$$\phi(S_1,S_2, \ldots ,S_{N-1},S_N) = (S'_1, \ldots ,S'_{N-1})$$

The cardinality of the set $\phi[(N)] \subseteq (N-1)$ does not exceed 2^{N-1}, clearly.

Moreover: $$\phi(\underline{S}) = \phi(-\underline{S}) \qquad (4.3.15)$$

as is seen by inspection , thus each image under ϕ has at least two preimages . Too , ϕ is onto, since for each $\underline{S}' \in (N-1)$ we can find, by construction if necessary, a preimage in (N) . And then we have necessarily two preimages by virtue of (4.3.15) . Finally, each vector in (N-1) has at most two preimages in (N) . To see this, we compare the components of the preimage vector giving:

$$S'_{j-1} = S_j S_{j-1} \quad \text{as the components of the image.}$$

Now the equation:

$$S''_j S''_{j-1} = S_j S_{j-1} \quad \text{has exactly two solutions,}$$

namely the ordered pair $\pm (S_j,S_{j-1})$, since the S's are restricted to ± 1 .

Hence each vector in (N-1) has exactly two preimages !

The correspondence ϕ is not one-one . Define as <u>upper half</u> and <u>lower half</u> of (N) the subsets: $(N)^+ = \{(S_1, \ldots ,S_{N-1},+1)\}$, $(N)^- = \{(S_1, \ldots ,S_{N-1},-1)\}$ respectively. Both subsets have the same cardinality, namely 2^{N-1}. Both subsets are equivalent in the set-theoretical sense.

Furthermore, if $\underline{S} \in (N)^+$, then $-\underline{S} \in (N)^-$, and vice versa.

Taking the results of our discussion together, we see that to each $\underline{S}' \in (N-1)$ there corresponds exactly one preimage in each of $(N)^+$ and $(N)^-$.

We have the set-theoretical equivalences:

$$(N)^+ \triangleq (N-1) \quad , \quad (N)^- \triangleq (N-1) \qquad (4.3.16)$$

We return to item (4.3.11a):

$$-\beta H(\underline{S}) = x \sum_{j=2}^{N} S_j S_{j-1} + y \sum_{j=3}^{N} S_j S_{j-2} \qquad (4.3.11a)$$

and rewrite this as: (on using the argument preceding (4.3.13))

$$-\beta H'\left[\phi(\underline{S})\right] = -\beta H'(\underline{S}') = x \sum_{j=1}^{N-1} S_j' + y \sum_{j=2}^{N-1} S_j' S_{j-1}'$$

which corresponds to (4.3.12a) . Accordingly we have for the summation over the upper half $(N)^+$:

$$\sum_{\underline{S} \in (N)^+} \exp(-\beta H(\underline{S})) = \sum_{\underline{S}' \in (N-1)} \exp(-\beta H'(\underline{S}'))$$

and likewise for the lower half , $(N)^-$. Since $(N) = (N)^+ \cup (N)^-$, and $(N)^+ \cap (N)^- =$ empty set , we have:

$$\sum_{\underline{S} \in (N)} \exp(-\beta H(\underline{S})) = 2 \sum_{\underline{S}' \in (N-1)} \exp(-\beta H'(\underline{S}'))$$

which proves (4.3.1o). QED.

Précis

The thesis is a study on the linear Ising model and the related linear lattice fluid.After a brief discussion of the relevant formulae from statistical mechanics we focus our attention almost exclusively on the two types of assembly.A methodology,using some aspects of set theory, is derived and then employed throughout the thesis.

We obtain and compare results for models with first and finite order interactions on the one hand,and models having modified long range interaction potentials on the other.The ferromagnetic behaviour of the straight line version of the linear model with simplified long range interaction potential is demonstrated with mathematical rigour whereby we use a result from the theory of measure and integration.By contrast,we show that the ring model with up to and inclusive second order interactions undergoes no spontaneous magnetisation.Then,on extending the matrix method employed for the second order case,we motivate the conjecture that finite order interaction potentials will not permit spontaneous magnetisation at finite and non-zero temperatures.This result agrees with a more general theorem on phase changes for one-dimensional assemblies.

We derive the closed form partition function for the straight line version of the linear lattice fluid having first order interaction potential only (square well potential) and then we use this function to obtain the partition function for an assembly having square well plus long range "tail" interaction potential.Again,in contrast to the former,the latter assembly can undergo a change of phase.The mathematical"mechanism"of this change of phase, if it occurs,is shown to be the modes of intersection of two "floating" curves. We consider this "mechanism" as rather interesting and,perhaps,novel. Using the same principles,we further propose a method by which the closed form partition function of an assembly having a finite range "step-potential" is employed to derive the closed form partition function for an assembly having the same finite range step-potential plus long range "tail" .

On using this method on the straight line version of the linear model with square well plus long range "tail" ,we again show the existence of ferromagnetism - this would be expected anyway - but the more interesting part of the result is that the critical temperature is now raised by a factor greater than 2 , using the same numerical value for the interaction potential.Our conclusion was that the addition of a realistic first order interaction potential to the long range "tail" increases the thermal stability of the magnetic structure of the assembly.

Finally,we develop,from first principles,an operator formulation for the linear Ising model and the related lattice fluid.The operator formulation can be extended to higher dimensions and applies equally well to periodic and non-periodic boundary conditions.We believe that the operator formulation is a novel approach to the Ising problem for arbitrary interactions.This principle is then employed to derive - in a brief and elegant manner - a recurrence relation for the straight line version's partition function,involving first order interactions in the presence of an external magnetic field. The recurrence relation was first published in 1968.

We conclude the thesis by stating and proving a curious little lemma for the partition function of the straight line model having interactions up to and inclusive second order in the presence of an external magnetic field.

Almost all of our work is built up right from first principles and based on the methodology set forth at the beginning of the thesis.Except for accepting the general formulation of the Ising problem,we have not sought to duplicate,or work in analogy to , results and methods already laid down in the current intermediate literature on the subject.In view of this,we ask for the readers understanding for our somewhat meagre list of references to published papers.

Reference on literature:

i) Quoted books and papers.

(I) : "Statistical Mechanics" , K.Huang , J.Wiley.

(II) : "Model of a cell fluid" ,Tross and Lund , JOURNAL OF MATH.PHYS. Vol.9 , No. 11 , November 1968.

(III) : "Linear Algebra" , Mirsky , Oxford.

(IV) : "Introduction to functional analysis" , A. Taylor , J.Wiley.

(V) : "Statistische Thermodynamik" , Münster , Springer.

(VI) : "The equilibrium theory of classical fluids" , Frisch and Lebowitz , Benjamin.

(VIII) : "Difference equation solution for the linear Ising model and nearest neighbour fluid" , Leff and Flicker, American Journal of Physics,July 1968.

(IX) : "Rekursive Folgen" , Markuschewitsch , Berlin .

(VII) : "Physical Chemistry" , Maron and Prutton , MacMillan.

ii) Collateral readings:

1) : "Statistische Physik" , Landau und Lifschitz , Berlin.

2) : "Theory of sets" , Kamke , Dover.

3) : "Handbuch der Physik" , Bände III/2 , XII , XIII . Flügge ,Springer.

4) : "Statistical Mechanics" , Khinchin , Dover.

5) : "Elementary principles of statistical mechanics" , Gibbs , Dover.

6) : "Thermodynamics" , E. Fermi , Dover.

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