RENORMALIZATION TECHNIQUES IN THE STUDY OF CRITICAL PHENOMENA

I : Lattices of Effectively Nonintegral Dimensionality

II : A Model of the Melting Transition

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Deepak Dhar

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To my parents

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ABSTRACT

This thesis is divided into two parts.

In Part I, we give an explicit construction for a class of lattices with effectively non-integral dimensionality. A reasonable definition of dimensionality applicable to lattice systems is proposed. The construction is illustrated by several examples. We calculate the effective dimensionality of some of these lattices. The attainable values of the dimensionality d , using our construction, are densely distributed in the interval $1<d<\infty$.

The variation of critical exponents with dimensionality is studied for a variety of Hamiltonians. It is shown that the critical exponents for the spherical model, for all d, agree with the values derived in literature using formal arguments only. We also study the critical behavior of the classical p-vector Heisenberg model and the Fortuin-Kasteleyn cluster model for lattices with $d<2$. It is shown that no phase transition occurs at nonzero temperatures. The renormalization procedure is used to determine the exact values of the connectivity constants and the critical exponents α, γ and ν for the self-avoiding walk problem on some multiply connected lattices with $d<2$. It is shown by explicit construction that the critical

exponents are not functions of dimensionality alone, but depend on detailed connectivity properties of the lattice.

In Part II, we investigate a model of the melting transition in solids. Melting is treated as a layer phenomenon, the onset of melting being characterized by the ability of layers to slip past each other. We study the variation of the root-mean-square deviation of atoms in one layer as the temperature is increased. The adjacent layers are assumed held fixed and provide an external periodic potential. The coupling between atoms within the layer is assumed to be simple harmonic. The model is thus equivalent to a lattice version of the Sine-Gordon field theory in two dimensions. Using an exact equivalence, the partition function for this problem is shown to be related to the grand partition function of a two-species classical lattice Coulomb gas. We use the renormalization procedure to determine the critical behavior of the lattice Coulomb gas problem. Translating the results back to the original problem, it is shown that there exists a phase transition in the model at a finite temperature T_c. Below T_c, the root mean square deviation of atoms in the layer is finite, and varies as $(T_c - T)^{-1/4}$ near the phase transition. Above T_c, the root mean square deviation is infinite. The specific heat shows an essential singularity at the phase transition, varying as $\exp(-|T_c - T|^{-1/2})$ near T_c.

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PART I

LATTICES OF EFFECTIVELY NONINTEGRAL DIMENSIONALITY

I : INTRODUCTION

In recent years much attention has been devoted to the study of the variation of critical exponents as a function of d, where d , the dimensionality of space , is treated as a continuously variable parameter. Nonintegral dimensions were first introduced to aid the understanding of critical phenomena exhibited by a binary fluid system of "Gaussian molecules" [1]. Wilson and Fisher [2-4] developed the technique called ε-expansion which allows one to write critical exponents for Ising-like models as power series in ε , where $\varepsilon=4-d$. These ε-expansion calculations have been pushed up to third order in ε by Brezin, Le Guillou, Zinn-Justin and Nickel [5-6]. Similar series expansions in powers of ε , where the space dimensionality is $2-\varepsilon, 2+\varepsilon, 6-\varepsilon$ etc. [7-12] have been developed to describe a wide variety of phase transitions in different physical systems. In quantum field theory [13-15], the space dimension $4-\varepsilon$ has been introduced to regularize the ultraviolet divergences in perturbation theory. Also atomic bound states have been studied as a function of continuously varying d [16].

Despite much work done dealing with the computational aspects of the ε-expansion techniques,(only some of which was cited above) its conceptual basis has remained quite obscure. Just what physical meaning may be assigned to

these ε-expansions ? We may argue that the appearance of ε as a continuous variable is a technical or mathematical artifice, and that physically meaningful results correspond only to integral values of ε . This argument fails , however , because the radius of convergence of these expansions (if they converge at all ; there are indications that the expansions are only asymptotic [17]) is expected to be much less than one. In the following , we shall attempt to answer this question by explicitly constructing a class of lattices having nonintegral dimensionality. These lattices are generalizations of the truncated tetrahedron lattice, invented by Nelson and Fisher [18].

The lattices are defined recursively. They are multiply connected and have some unusual topological properties. In particular, they are spatially inhomogenous and highly anisotropic. They may be called pseudo-lattices to distinguish them from the "regular" lattices usually encountered in solid state theory or statistical physics.

An example of a pseudo-lattice is the Bethe lattice , which has been very important historically in the development of the theory of phase transitions. Detailed study of the Ising model on this lattice has suggested the possibility of a new class of phase transitions (phase transitions of continuous order)[19] , which have subsequently been realized on more conventional lattices

[20].

Part of the motivation for the study of these pseudo-lattices springs from the fact they are very good pedagogical examples of renormalization group techniques at work . Despite enormous progress in the application of the renormalization group to the field of phase transitions since the pioneering work of Kadanoff and Wilson [21], the number of cases showing nontrivial phase transitions where the exact renormalization transformation may be explicitly implemented has remained rather small . The only other exceptions are the Gaussian model [22] and the hierarchical model [23]. These lattices may also be used to test the validity of new approximation schemes .

While , as explained above , the ε-expansion techniques have motivated and influenced our analysis , a familiarity with them is not a prerequisite for an understanding of the ensuing discussion . Indeed, the major goal of this half of our thesis is to provide an explicit construction of lattices of effectively nonintegral dimensionality , where the critical behavior of various Hamiltonians may be explicitly determined independently of the ε-expansion techniques, and thus provide a "reason for existence " and testing grounds for these techniques . Some previous exposure to the renormalization group formalism will be helpful in following the arguments, but it is not necessary.

II : OUTLINE

The discussion is organized as follows:

In Section III we define what we mean by the effective (nonintegral) space dimensionality of an infinite lattice . The dimension of a lattice is defined in terms of the density of states of the low frequency modes for a nearest neighbour harmonic interaction Hamiltonian on the lattice. The proposed definition is different from that assumed by Nelson and Fisher [18]. In particular the space dimensionality of the truncated tetrahedron lattice using our definition is found to be $2 \log_5 3 \approx 1.3652$, and not $\log_2 3 \approx 1.5850$ as proposed by Nelson and Fisher. Arguments are presented in favor of our definition.

In Section IV we give some examples of lattices having nonintegral values of effective dimensionality. One is a generalization of the truncated tetrahedron lattice to the truncated n-simplex lattice. We define the (M,N) modified rectangular lattice and the $(M,N)_r$ modified rectangular lattice. Here M and N are arbitrary positive integers. The (M,N) modified rectangular lattice , and the $(M,N)_r$ modified rectangular lattices are planar , multiply connected lattices with coordination number 3 or 4. These lattices may be obtained by selectively deleting some bonds from a

two dimensional rectangular lattice. We also define a modified n-cuboid lattice . Other lattices of this type are easy to construct. The effective dimensionalities of some representative cases of these lattices are determined in Section V by deriving functional equations for their characteristic functions and determining their frequency spectra.

In Section VI , the critical behavior of the spherical model on a d-dimensional lattice is outlined , for arbitrary d. We give the expressions for critical exponents as functions of d . It is shown that the critical exponents are piecewise continuous functions of d . We also verify that all the various critical exponents that may be defined are not independent , and simple relations exist amongst them .

The spherical model is exceptional in that its critical behavior can be analysed for arbitrary dimension d . This is not true for most Hamiltonians, where no simple separation of variables takes place . In the next three sections we consider some of these cases. Section VII contains a discussion of the classical p-vector Heisenberg model . In Section VIII we discuss the Fortuin-Kasteleyn cluster model. The behavior of these models has been determined only for $d<2$. For $d<2$, due to the special structure of these lattices, we can write down the exact

renormalization equations in terms of a finite number of coupling constants . For simplicity, we shall consider only the truncated tetrahedron lattice . Other lattices may be similarly treated , and so long as d<2, the qualitative behavior of these lattices is quite similar and is characterized by the absence of a phase transition at nonzero temperatures. We determine the behavior of correlations in these models at very low temperatures. It is found that the susceptibility of the p-vector model varies as the $(\frac{2}{2-d})^{th}$ power of the inverse temperature . The correlations are much stronger in the cluster model, and there the mean size of a cluster varies as an exponential of an exponential of the inverse temperature . Lattices with d>2 are much more interesting, because they show phase transitions ; but then the renormalization equations become much more complicated and are difficult to analyse .

In Section IX , we discuss self avoiding random walk problems. These walks show a nontrivial phase transition for multiply connected lattices, in the sense that the generating functions of the random walk become singular as functions of their argument. The nature of the singularity and the values of the critical exponents α, γ and ν are determined for the truncated tetrahedron lattice, the truncated 4-simplex lattice, and the $(2,1)_p$ modified rectangular lattice .

In this case , however , no simple expressions exist for the critical exponents as functions of the dimensionality of the lattice . In fact, we can construct examples of lattices that have the same space dimensionality, but different critical exponents α, γ and ν. It is suggested that this is because the asymptotic behavior of self avoiding random walks depends on detailed connectivity properties of the lattice and not on the dimensionality alone . We conclude with some final remarks in Section X .

III: DEFINITION OF THE SPACE DIMENSIONALITY OF AN INFINITE LATTICE

Consider an infinite lattice. For our purpose a lattice is specified by its graph consisting of lattice points and lines joining them called bonds. For simplicity we consider only one kind of bonds. Two sites that have a bond in common are called nearest neighbours . How do we assign a dimensionality to an arbitrary infinite lattice ? (The effective dimensionality of a finite lattice may be defined to be zero.) Any proposed definition of effective dimensionality should satisfy some elementary properties. It should agree with the conventional integral value of dimensionality for "regular " lattices . It should depend only weakly on the lattice in the sense that introduction or deletion of a finite number of lattice points or bonds should not change its value. And preferably it should satisfy some scaling relations between critical exponents [24].

It is instructive to look at the familiar case when the space dimensionality d is integral. We consider a "simple cubic " lattice in d dimensions and consider a model in which a scalar displacement X_i is associated with each site i and nearest neighbours are connected by harmonic springs of equal spring constants. Introduction of normal mode

coordinates converts this problem into one of independent simple harmonic oscillators . Each normal mode is characterized by a wave number $\vec{K}$ which is a d-dimensional vector lying within the first Brillouin zone. We also know that :

(i) For small wavenumbers, the frequency ω of the mode with wave number $\vec{K}$, is approximately proportional to the magnitude of $\vec{K}$, i.e. , $\omega^2 = K^2 C^2$ for small $|\vec{K}|$.

(ii) The number of modes with $|\vec{K}| < K_c$ is proportional to K_c^d for small K_c. These two facts together imply that the fractional number of modes with frequency less than ω is proportional to ω^d for small ω .

In making a transition to more general lattices with possibly nonintegral dimensionality , we may again define a nearest neighbour harmonic interaction model . It is difficult to say just what meaning may be assigned to a "non integral-dimensional vector $\vec{K}$". At best, we may say that low values of $|\vec{K}|$ correspond to slow space varying modes and large value of $|\vec{K}|$ correspond to modes where the spatial variation is large . We necessarily assume that something like (ii) is correct. Compare this , for instance , with the scaling property assumed by Wilson (Eq.(A3) and (A9) in Ref. [25]).

The validity of (i) is rendered plausible by the observation that the equation $\omega^2 = K^2C^2$ is just the Fourier transform of the equation $\frac{\partial^2 \chi}{\partial t^2} = C^2 \nabla^2 \chi$. If we identify χ_i as the displacement at site i and replace $\nabla^2 \chi$ by its discrete analog $\sum_j (\chi_j - \chi_i)$ where j are the sites neighbouring i, we see that the equation correctly gives the equation of motion of χ_i in our model.

It is thus reasonable to postulate that the fractional number of modes with frequency less than ω is proportional to ω^d, for small ω, even if d is nonintegral. We adopt this as the definition of effective dimensionality of an infinite lattice.

In practice, the determination of the fractional number of modes below a frequency ω involves starting with a finite lattice of size N, and then letting N tend to infinity. For an arbitrary lattice such a limit obviously does not exist. In statistical mechanics we shall only be concerned with lattices which are sufficiently regular and all such limits will be assumed to exist.

Analysis given in Section V shows that the effective dimensionality of the truncated tetrahedron lattice is $2 \log_5 3$.

Nelson and Fisher give a different argument to determine the effective dimensionality. We give here a somewhat more careful formulation of their reasoning applicable to infinite lattices. Define the distance between two lattice points of a lattice as the minimum number of bonds that have to be traversed in order to go from one point to the other. A sphere of radius R (here R is an integer) about a point C, is the set of points whose distance from the point C, called the center of the sphere , is less than or equal to R. The volume of a sphere is the number of points inside it . We average over all positions of the center to define the average volume $\overline{V}(R)$ of a sphere of radius R, which is independent of the location of the center. The dimensionality of the lattice may be defined by

$$d = \lim_{R\to\infty} \frac{\ln \overline{V}(R)}{\ln R} \quad . \tag{1}$$

In mathematics literature, this is called the Hausdorf dimensionality of the space. Using this procedure, the dimensionality of the truncated tetrahedron lattice may be shown to be $\log_2 3$. This follows trivially from the inequalities $2.3^r \geq \overline{V}(2^r) \geq 3^r$.

The two definitions of dimensionality are clearly not equivalent , as they give different values for the dimensionality of the truncated tetrahedron lattice. The important difference is that while in Nelson and Fisher's definition one considers the lattice as a whole, our

proposed definition looks only at the low spatial frequency modes. Since phase transitions are governed by the long-range correlations, i.e. low frequency modes, we believe that our proposed definition is more relevant to the study of phase transitions.

For example , the $(2,1)_p$ modified rectangular lattice, defined in the next section , has an effective dimensionality 3/2 using our definition. If we use Nelson and Fisher's definition , the effective dimensionality of the lattice would be 2. However, the behavior of model Hamiltonians like the Gaussian model or the Ising model on this lattice is very different from that on a two dimensional square lattice. In particular, it may be shown that on this lattice, the Ising model shows no spontaneous magnetization or phase transition. Thus we may expect the assigned effective dimensionality to be less than two. Similar argument may be made for the truncated n-simplex lattice.

We note that the effective dimensionality of a lattice has been defined in terms of a specific model (nearest neighbour harmonic spring interaction model). We expect the dimensionality of a lattice to be model independent and different definitions of effective dimensionality using other model Hamiltonians should give identical value of dimensionality when it is calculated correctly in terms of

independently determinable critical exponents of the model. The quadratic Hamiltonian was chosen due to its simplicity.

In particular, the dimensionality of a lattice would not change if we introduced a second nearest neighbour spring interaction , or any quadratic interaction of finite range for that matter. This may be proved rigorously using the exact renormalization equations, but is most easily seen by the application of first order perturbation theory. Let the first and the second nearest neighbour spring constants be J and J' respectively, J'<<J. The change in ω_i^2, the frequency of the i^{th} mode is given by

$$\frac{d\omega_i^2}{dJ'} = \alpha \omega_i^2 + \text{higher order terms in } \omega_i. \qquad (2)$$

where α is some constant depending on the lattice. This implies that the power law dependence of the density of states in the low frequency region remains unchanged.

Finally , we mention the works of Wilson [25], Stillinger [26], and Mendelbrot [27], who have also studied spaces of nonintegral dimensionality . Wilson and Stillinger have developed their ideas starting from a set of axioms that are assumed to hold for the spaces in question. While they give explicit rules for the calculation or various integrals in such spaces, they do not give any concrete examples. Also, their axioms hold for continuum spaces and the generalization to discrete spaces is not

straightforward (if possible) . This is a great disadvantage in statistical physics and field theory, where the lattice formulations are much easier to handle as the infinities associated with small scale behavior are avoided.

Vector addition is allowed in Wilson's axioms . This implies the existence of a denumerable (finite or infinite) set of basis vectors . The number of such basis vectors, inevitably , becomes the dimension of the space for most purposes . While Stillinger explicitly rejects vector addition in his formulation, he introduces an axiom concerning the behavior of Gaussian integrals in his space, which implies non-positivity of the integration measure in the space . Expressed more simply, the axioms imply that the "volume" of some set of points has to be negative . This is a very serious drawback, because the proofs of many existence theorems that form the foundations of statistical physics (e.g. the existence of a thermodynamic limit, convexity of the free energy etc.) fail to hold in such a case. Also Stillinger's definition of dimensionality of the space is the same as Nelson and Fisher's discussed above, and the same arguments apply to this case .

Mendelbrot's definition of objects of nonintegral dimensionality, called fractals, assumes the existence of an underlying space of integral dimensions. The dimensionality of fractals is defined in terms of the change in volume of

these fractals under a magnification or contraction of the underlying integral dimensional manifold. For instance, the dimensionality of a line is related to its "kinkiness" in an underlying two dimensional space . This definition of effective dimensionality does not seem to be very useful in statistical physics or field theory . In any case, the assigned numerical value of the dimensionality for fractals is the same as given by Eq.(1). Hence the arguments agaist the definitions of Wilson, Stillinger, Nelson and Fisher extend to this case as well. We shall not discuss it any further here .

IV : SOME EXAMPLES OF LATTICES WITH NONINTEGRAL DIMENSIONALITY

In this section we describe some examples of lattices with nonintegral effective dimensionality . The lattices are defined recursively in such a way that the exact renormalization equations for Hamiltonians on these lattices may be written down explicitly in terms of a small (usually finite) number of coupling constants. It is easy to construct other lattices of this type .

A : The Truncated n-Simplex Lattice

The truncated n-simplex lattice is a simple generalization of the truncated tetrahedron lattice. The lattice is defined recursively. The graph of the zeroth order truncated n-simplex lattice is a complete graph on (n+1) points. (A complete graph is a graph in which there

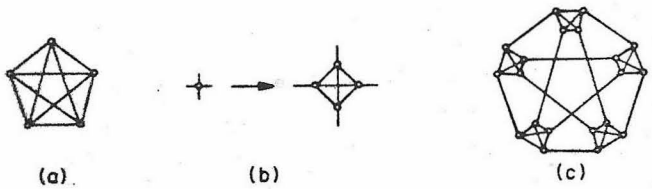


FIG. 1. (a) A complete graph on 5 points, zeroth order truncated 4-simplex lattice. (b) Replacement of single vertex by a complete 4 point graph. (c) Result of replacement on Fig. (a). First order truncated 4-simplex lattice.

exists a bond between every pair of points.) The graph of the (r+1)th order lattice is obtained by replacing each of the vertices of the rth order graph by a complete graph on n points. Each of the new n points is connected to one of the lines coming to the original vertex. For the thermodynamic limit, we let r tend to infinity. In Figure 1 the construction is illustrated for the case n=4.

The case n=1 corresponds to the uninteresting case of mutually disconnected pairs of points. n=2 corresponds to a linear chain . For n=3 , we get the truncated tetrahedron lattice . For higher values of n the lattices are nonplanar. It is easy to see that the rth order truncated n-simplex lattice has $(n+1)n^r$ vertices and $(n+1)n^{r+1}/2$ bonds. The coordination number of each lattice point is n . While the lattice is multiply connected for n>2 , it is possible to disconnect an arbitrarily large set of points from the rest of the lattice by deleting only n bonds. We show later that the effective dimensionality of this lattice is $(2 \log n)/\{\log(n+2)\}$.

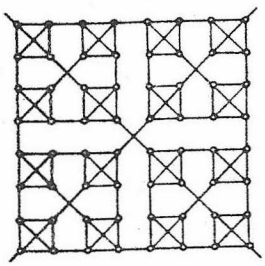


FIG. 2. A portion of the infinite truncated 4-simplex lattice.

The truncated 4-simplex lattice may be more conveniently drawn as in Fig.2 as a square lattice with bonds connecting at most "next nearest neighbors". The quotation marks indicate that the word is used in the Euclidean sense. By our definition all pairs of points having a bond in common are nearest neighbors. The construction of the graph is explained in Fig.3. We define a first order square as a complete graph on four points. An $(r+1)^{th}$ order square is obtained by joining four r^{th} order squares together by bonds such that each r^{th} order square is

FIG. 3. (a) Graph of a first order square. (b) Schematic representation of the graph of the $(r+1)$th order. The shaded squares denote the graph of rth order squares of which only the corner vertices are shown.

joined to the other r^{th} order squares by bonds connecting corner points, and each r^{th} order square contributes one corner point to the $(r+1)^{th}$ order square. The graph in Fig.2 is a third order square. It is easy to convince oneself that the graph of the infinite order square is topologically equivalent to the graph of the infinite truncated 4-simplex lattice. Thus we may generate the truncated 4-simplex lattice from the graph of a two dimensional infinite square lattice with "nearest neighbor"

and "next nearest neighbor" bonds by selectively deleting some bonds. This deletion of bonds results in a change in the effective dimensionality of the lattice from 2 to 2 ln4/(ln6).

B : The (M,N) Modified Rectangular Lattice

For arbitrary positive integers M and N , the lattice is defined recursively as follows: The first order rectangle is a cyclic graph on four points. (A cyclic graph is a connected graph in which every point has two nearest neighbors.) To construct a graph of $(r+1)^{th}$ order , we take MN r^{th} order rectangles and arrange them in an M×N array.

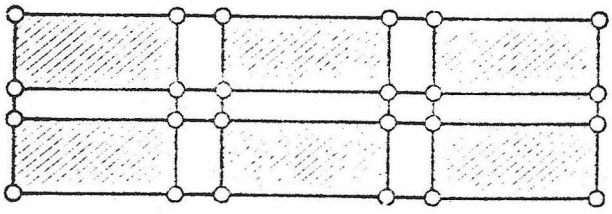


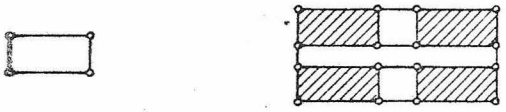
FIG. 4. A schematic representation of the graph of the (r+1)th order rectangle of the (2,3) modified rectangular lattice. The shaded rectangles are the graphs of rth order rectangles of which only the corner vertices are shown.

We connect these rectangles by introducing additional vertical and horizontal bonds to join the corner vertices of all the adjacent rectangles. No additional bonds are added to any vertex that is not a corner vertex of any r^{th} order rectangle. In all we add 2M(N-1) horizontal bonds and 2N(M-1) vertical bonds. The resultant figure defines a (r+1)th order rectangle. Clearly the (r+1)th order rectangle has $4M^rN^r$ vertices . The lattice is planar and all the vertices have coordination numbers 3 or 4. Fig.4 illustrates the construction for the case M=2,N=3.

The procedure of determining the effective dimensionality, to be discussed in the next section, may be applied to this lattice as well. For arbitrary M and N, however, the resulting equations are quite complicated (though there are only a finite number of them involving only rational functions) , and an explicit expression for dimensionality in terms of M and N is difficult to obtain. It is however easy to see that for M=N=1, the lattice is finite and hence zero dimensional. If N=1, and M>1, the lattice is one dimensional. For M>1 and N>1 , the effective dimensionality of the lattice is between 1 and 2. By an appropriate choice of integers M and N , a lattice with effective dimensionality arbitrarily close to any preassigned value between 1 and 2 may be obtained.

C : The $(M,N)_r$ Modified Rectangular Lattice

The construction of this lattice is very similar to that of the (M,N) modified rectangular lattice, except for the fact that we rotate the r^{th} order rectangles by 90° after arranging them to form the M x N array to form the $(r+1)^{th}$ order rectangle. The subscript r stands for rotation. The effect of this rotation is to reduce the anisotropy of the lattice. The ratio of the "length " and the "width" of the r^{th} order rectangle does not increase as $(M/N)^r$, as in the



(a) (b)

FIG. 5. (a) The graph of the first order rectangle. (b) Schematic representation of the graph of the (r+2)th order rectangle of the $(2,1)_r$ modified rectangular lattice. The shaded areas denote graphs of rth order rectangles of which only the corner vertices are shown.

previous case , but remains finite for all r. It is M/N if r is even, and 1 if r is odd.

Like the (M,N) modified rectangular lattice, this lattice is planar and may be obtained from a two dimensional square lattice by selectively deleting some bonds. The simplest example of this class is the case M =2 , N = 1. Since the values of M and N are low, the recursion equations for this case are usually quite easy to write down. The construction is illustrated in Fig. 5. In the next section we show that the effective dimensionality in this case is 3/2.

D : The Modified n-Cuboid Lattice

We may similarly define a modified n-cuboid lattice. The n-cuboid is an n-dimensional generalization of a rectangle (n is a positive integer) . The first order n-cuboid graph has 2^n points. Each point has n neighbors and the graph has nearest neighbor relations and the symmetry of an n-dimensional cuboid. The (r+1)th order graph is obtained by bringing together two rth order graphs and connecting the 2^{n-1} corner vertices on one "(n-1) dimensional face" of one r^{th} order cuboid to the corresponding 2^{n-1} corner vertices of the other cuboid with 2^{n-1} bonds. The result is a graph of an (r+1)th order cuboid whose corner vertices are the $2^{n-1} + 2^{n-1}$ corner vertices of the starting set which were not connected

together. This procedure of "glueing" together of cuboids is done cyclically in the n different directions along the axes of the cuboids. Using the same techniques as developed in the next section, it may be shown that the effective dimensionality of this lattice is $2(1-2^{-n})$. The $(2,1)_n$ modified rectangular lattice corresponds to the special case n=2. The details of the calculation are of marginal interest only and are omitted here.

By varying n in the truncated n-simplex lattice , we get lattices of effective dimensionality 0, 1, $2\log_5 3$, $2\log_6 4$,... With the proper choice of the integers M and N , we may get an effective dimensionality arbitrarily close to any preassigned value between 1 and 2 , from examples B and C. The effective dimensionality of the lattice is, however, always less than two. The same is true of example D. It is, however, easy to obtain lattices of higher dimensionality. Given two lattices L_1 and L_2, we define their direct product lattice $L = L_1 \times L_2$ as follows: For each ordered pair (ℓ_1, ℓ_2), where ℓ_1 and ℓ_2 are any lattice points in the lattices L_1 and L_2 respectively, we associate a unique lattice point $\ell \in L$. The points $\ell, \ell' \in L$, where $\ell=(\ell_1, \ell_2)$, $\ell'=(\ell_1', \ell_2')$, are nearest neighbors of each other in L iff

(i) $\ell_1 = \ell_1'$ and (ℓ_2 and ℓ_2' are nearest neighbors in L_2) or

(ii) $\ell_2 = \ell_2'$ and (ℓ_1 and ℓ_1' are nearest neighbors in L_1).

It is easy to see that the effective dimensionality of L is the sum of the effective dimensionalities of L_1 and L_2. For example, the direct product of a linear chain and a square lattice is a simple cubic lattice of dimensionality 3=1+2.

This gives us a whole class of lattices with effectively nonintegral dimensionality, so that the effect of changing dimensionality on the critical exponents etc. , may be studied in much more detail than has been possible so far. By forming the direct product of the $(2,1)_\gamma$ modified rectangular lattice with itself, we get a lattice of effective dimensionality 3. Verification that the critical exponents for, say, the Ising model on this lattice are the same as for the simple cubic lattice would be an important test of the usefulness and relevance of our definition of dimensionality, and of the strength of the universality hypothesis.

V : DETERMINATION OF THE EFFECTIVE DIMENSIONALITY

We now show how the effective dimensionality of the recursively defined lattices, examples of which were described in the previous section , may be determined. For simplicity, we discuss only the cases of the truncated n-simplex lattice and the $(2,1)_r$ modified rectangular lattice. The truncated n-simplex lattice is discussed in some detail . It has relatively simple recursion equations involving only one variable. We analyse the spectrum in some detail to familarize ourselves with the renormalization group techniques. The $(2,1)_r$ modified rectangular lattice is discussed to illustrate how the effective dimensionality may be determined when the recursion equations involve more than one variable.

The same technique is applicable to other recursively defined lattices, though the analysis of the recursion equations is usually more involved. We use the renormalization transformation to determine the frequency spectrum of the nearest neighbour Hamiltonian on the lattice. In general, for $1<d<2$, the frequency spectrum is quite singular and consists of an infinite number of delta functions of varying heights. The dimensionality of the lattice is deduced from the power law behavior of the

cumulative frequency distribution function for low frequencies. The procedure is equivalent to determining the low temperature specific heat behavior of a Debye solid on the lattice. If the low temperature specific heat is proportional to T^d, where T is the temperature, we identify d as the effective dimensionality of the lattice.

A. The Truncated n-Simplex Lattice

We define the spherical model on this lattice by assigning a continuous spin χ_i $(-\infty<\chi_i<+\infty)$ to each of the sites i of the r^{th} order truncated n-simplex lattice. The index i goes from 1 to $N_r=(n+1)n^r$. The nearest neighbour sites are assumed to have a ferromagnetic Ising interaction of strength J. The spherical constraint $(\sum_i \chi_i^2 = N)$ is taken care of by introducing a Lagrange parameter λ in the Hamiltonian, so that the Hamiltonian of the system is

$$H = (J/2) \sum_{\text{nearest neighbours } (i,j)} (\chi_i - \chi_j)^2 + (\lambda J/2) \sum_i \chi_i^2 \,. \qquad (3)$$

We get the partition function as

$$Z_r(\lambda) = \prod_i \left(\int_{-\infty}^{+\infty} d\chi_i \right) \exp(-\beta H) \,, \qquad (4)$$

where β is the inverse temperature. This is a Gaussian integral and may be done easily, giving

$$Z_r(\lambda) = (2\pi/\beta J)^{N_r/2} G_r(\lambda) \tag{5}$$

with

$$G_r(\lambda) = \prod_{i=1}^{N_r} (\omega_i^2 + \lambda)^{-1/2} , \tag{6}$$

where ω_i^2 are the normal mode frequencies of the model. The treatment of this model is quite parallel to that of the Ising model discussed in Ref. [18]. In particular we may define the analogs of the star triangle and the dedecoration transformations in the continuous spin case. These transformations follow from the identities

$$\exp\left[-\tfrac{1}{2}\sum_{i,j=1}^{n}(x_i - x_j)^2\right] = n\int_{-\infty}^{+\infty}\frac{dy}{\sqrt{2\pi}}\exp\left[-\frac{n}{2}\sum_{i=1}^{n}(y-x_i)^2\right] , \tag{7}$$

$$\int_{-\infty}^{+\infty}\frac{d\xi}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\frac{d\eta}{\sqrt{2\pi}}\exp\left[-\frac{n}{2}(x_1-\xi)^2 - \frac{\lambda}{2}\xi^2 - \tfrac{1}{2}(\xi-\eta)^2 - \frac{\lambda}{2}\eta^2 - \frac{n}{2}(\eta-x_2)^2\right]$$

$$= (\lambda+n)^{-1/2}(\lambda+n+2)^{-1/2}\exp\left[\frac{-n^2(x_1-x_2)^2}{2(\lambda+n)(\lambda+n+2)} - \frac{n\lambda(x_1^2+x_2^2)}{2(\lambda+n)}\right] . \tag{8}$$

These identities are applied as follows: We group the N_r spins into N_r/n groups of n spins each , such that each spin interacts with every other spin in the same group with

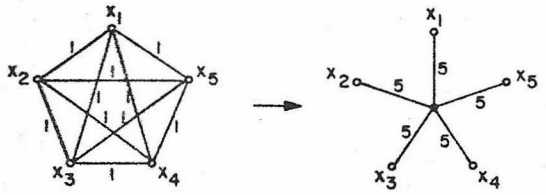


FIG. 6. An example of the generalized star triangle transformation with $n = 5$.

interaction strength 1 in scaled units. Then we introduce a

new spin y_j for each group j and couple it to each of the spins in its group with interaction strength n. The original n(n-1)/2 bonds within each group are deleted and replaced by n new bonds all connecting the new spin y_j to the other spins (Fig. 6). Identity (7) ensures that the partition function remains unchanged.

The second identity corresponds to the dedecoration transformation of Fisher (Fig. 7). We integrate over all the original spins x_i. This leaves us with the new spins y_j which form a $(r-1)^{th}$ order truncated n-simplex lattice, and all the spins y_j interact with their nearest neighbors on this lattice with a quadratic interaction. By a scale transformation on the spins y_j, this new interaction may be converted into an interaction of unit strength.

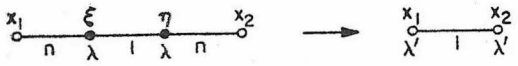


FIG. 7. The dedecoration transformation. Spins ξ and η are integrated over.

Applying these transformations we find that

$$G_n(\lambda) = [(\lambda+n)(\lambda+n+2)]^{-\frac{N_2}{4}+\frac{N_3}{2n}} G_{r-1}(\lambda^2+2\lambda+n\lambda). \qquad (9)$$

Define

$$F(\lambda) = \lim_{r\to\infty} \ln G_r(\lambda)/N_r \ . \qquad (10)$$

We get

$$F(\lambda)=-(n-2)/(4n)\ \ln[(\lambda+n)(\lambda+n+2)] + (1/n)F(\lambda^2+n\lambda+2\lambda). \qquad (11)$$

The frequency spectrum of the model may be determined from this functional equation for the characteristic function $F(\lambda)$. Details of the calculation are given in Appendix A. We note that $\lambda=0$ is a fixed point of the transformation . From Eq.(11) , putting $\lambda=0$, we get

$$F(0) = -[(n-2)/\{4(n-1)\}]\ \ln\ [n(n+2)]. \qquad (12)$$

From Eq.(A1) of the Appendix A , it is easily seen that for small $\lambda>0$, $F(\lambda)$ has an asymptotic expansion of the form $F(\lambda)= F(0) +A\lambda^{d/2} +$(higher order terms in λ), where d is the dimensionality of the lattice. Substituting in Eq.(11) and comparing the leading power of λ we get

$$A = (A/n)\ (n+2)^{d/2} \ . \qquad (13)$$

This implies that

$$d = 2\ \ln(n)\ /\ \ln(n+2) \ . \qquad (14)$$

It is interesting to note that this result may be obtained without the complicated analysis of Eq.(11) given in the Appendix.

B. The $(2,1)_r$ Modified Rectangular Lattice

For this lattice we wish to determine a functional equation of the same general form as Eq.(11) from which tne dimensionality of the lattice may be deduced. The functional equation is, however, much more complicated and involves five variables instead of one.

We have

$$H = (J/2)\sum_{(ij)} (\chi_i - \chi_j)^2 + (\lambda J/2)\sum_i \chi_i^2 , \qquad (3)$$

where the sum over (ij) extends over all nearest neighbor pairs (ij). We consider a more general form of the Hamiltonian and allow different interaction strengths and next-nearest neighbor interaction between spins belonging to the same first order rectangle. we write

$$H = (1/2)\sum_{ij} J_{ij} (\chi_i - \chi_j)^2 + (\lambda J/2)\sum_i \chi_i^2 , \qquad (15)$$

where J_{ij} =0 unless and are nearest neighbors or they belong to the same first order rectangle. J_{ij} may take four

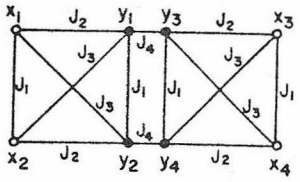


FIG. 8. Coupling constants for the modified rectangular lattice. The spins y_1, y_2, y_3, y_4 are integrated over.

different values J_1, J_2, J_3 or J_4. These interactions are depicted in Fig.(8) . J_1 , J_2 , J_3 are respectively the vertical, horizontal and diagonal bond strengths if i and j

belong to the same first order rectangle. J_4 is the interaction strength if i and j are nearest neighbors but do not belong to the same first order rectangle.

The renormalization transformation consists of integrating over the spins Y_1, Y_2, Y_3, and Y_4 and similar spins on other rectangles. This reduces the number of degrees of freedom in the Hamiltonian by a factor 2. The spins X_i, and similar spins on other rectangles again form the vertices of a $(2,1)_r$ modified rectangular lattice. The integrations over Y_i (i =1 to 4) give us an effective interaction between X_i (i = 1 to 4) and since the interaction is quadratic , it may again be expressed in the same form as Eq.(15) except for new values of the coupling constants J_1 , J_2 , J_3 . The value of J_4 remains unchanged. The most general form of the weight of an r^{th} order rectangle with corner spins X_1, X_2 , Y_1 , Y_2, and all other spins integrated over is

$$W^{(r)}(X_1,X_2;Y_1,Y_2) = C^{(r)} \exp\left[-\frac{\beta J_1^{(r)}}{2}\{(X_1-X_2)^2+(Y_1-Y_2)^2\} - \frac{\beta J_2^{(r)}}{2}\{(X_1-Y_1)^2+(X_2-Y_2)^2\} \right.$$
$$\left. -\frac{\beta J_3^{(r)}}{2}\{(X_1-Y_2)^2+(Y_1-X_2)^2\} - \frac{\lambda^{(r)}\beta J}{2}\{X_1^2+X_2^2+Y_1^2+Y_2^2\} \right] \quad (16)$$

We also have the recursion equation (Fig. 8)

$$W^{(r+1)}(X_1,X_3;X_2,X_4) = \int_{-\infty}^{+\infty}\int\int\int dY_1\,dY_2\,dY_3\,dY_4 \; W^{(r)}(X_1,X_2;Y_1,Y_2)$$
$$\cdot\, W^{(r)}(Y_3,Y_4;X_3,X_4) \cdot \exp\left[-\frac{\beta J_4}{2}\{(Y_1-Y_3)^2+(Y_2-Y_4)^2\}\right]. \quad (17)$$

The integrations in this equation are Gaussian and may be carried out easily. This gives us the recursion equations for the new coupling constants

$$C^{(r+1)} = (C^{(r)})^2 (2\pi)^2 \beta^{-2} (\lambda^{(r)} J + J_2^{(r)} + J_3^{(r)})^{-1/2} \times (\lambda^{(r)} J + 2J_1^{(r)} + J_2^{(r)} + J_3^{(r)})^{-1/2} \times (\lambda^{(r)} J + 2J_1^{(r)} + J_2^{(r)} + J_3^{(r)} + 2J_4)^{-1/2} , \quad (18a)$$

$$\lambda^{(r+1)} = \lambda^{(r)} (\lambda^{(r)} J + 2J_2^{(r)} + 2J_3^{(r)}) (\lambda^{(r)} J + J_2^{(r)} + J_3^{(r)})^{-1} , \quad (18b)$$

$$\lambda^{(r+1)} J + 2J_1^{(r+1)} + 2J_3^{(r+1)} = \lambda^{(r)} J + J_2^{(r)} + J_3^{(r)} - (J_2^{(r)} + J_3^{(r)})^2 (\lambda^{(r)} J + 2J_4 + J_2^{(r)} + J_3^{(r)})^{-1} , \quad (18c)$$

$$\lambda^{(r+1)} J + 2J_2^{(r+1)} + 2J_3^{(r+1)} = (\lambda^{(r)} J + 2J_1^{(r)} + 2J_3^{(r)}) (\lambda^{(r)} J + 2J_1^{(r)} + 2J_2^{(r)}) \times (\lambda^{(r)} J + 2J_1^{(r)} + J_2^{(r)} + J_3^{(r)})^{-1} , \quad (18d)$$

$$\lambda^{(r+1)} J + 2J_1^{(r+1)} + 2J_2^{(r+1)} = [(\lambda^{(r)} J + 2J_1^{(r)} + 2J_3^{(r)}) (\lambda^{(r)} J + 2J_1^{(r)} + 2J_2^{(r)}) + 2J_4 (\lambda^{(r)} J + 2J_1^{(r)} + J_2^{(r)} + J_3^{(r)})] [\lambda^{(r)} J + 2J_4 + 2J_1^{(r)} + J_2^{(r)} + J_3^{(r)}]^{-1} . \quad (18e)$$

Let the free energy per spin of the Hamiltonian given by Eq.(15) be $F(J_1, J_2, J_3, J_4, \lambda)$. From the renormalization transformation we get the equation

$$F(J_1, J_2, J_3, J_4, \lambda) = (1/8) \ln [C^{(r+1)} / C^{(r)^2}] + (1/2) F(J_1', J_2', J_3', J_4, \lambda') , \quad (19)$$

where $J_1', J_2', J_3', \lambda'$ are given by Eqs.(18b-e). To get the free

energy per spin of the original model we set $J_1 = J_2 = J_4 = J$ and $J_3 = 0$. We note that $\lambda = 0$ is a fixed point of the renormalization transformation . The free energy per spin is a singular function of λ near $\lambda = 0$ and has an asymptotic expansion of the form ($\lambda > 0$)

$$F(J_1, J_2, J_3, J_4, \lambda) = F(J_1, J_2, J_3, J_4, 0) + \lambda^{d/2} G(J_1, J_2, J_3, J_4) + \text{higher order terms in } \lambda . \quad (20)$$

We wish to determine the behavior of F for small λ. However, the value of $\lambda^{(r)}$ increases with iteration approximately as $\lambda^{(r+1)} \approx 2\lambda^{(r)}$ as is evident from Eq.(18b). Also the values of $J_1^{(r)}$, $J_2^{(r)}$, $J_3^{(r)}$ decrease with iteration. We choose initial λ sufficiently small and r sufficiently large so that

$$\lambda^{(r)} J << J_1^{(r)}, J_2^{(r)}, J_3^{(r)} << J_4 . \quad (21)$$

Then the recursion equations (18) may be approximated as

$$\lambda^{(r+1)} \approx 2\lambda^{(r)}, \quad (22a)$$

$$J_1^{(r+1)} + J_3^{(r+1)} \approx (1/2)(J_2^{(r)} + J_3^{(r)}), \quad (22b)$$

$$J_2^{(r+1)} + J_3^{(r+1)} \approx 2(J_1^{(r)} + J_2^{(r)})(J_1^{(r)} + J_3^{(r)})(2J_1^{(r)} + J_2^{(r)} + J_3^{(r)})^{-1}, \quad (22c)$$

$$J_1^{(r+1)} + J_2^{(r+1)} \approx J_1^{(r)} + (1/2)J_2^{(r)} + (1/2)J_3^{(r)} . \quad (22d)$$

Now, if we write $F^{singular}(J_1, J_2, J_3, J_4, \lambda)$ as the singular part of the free energy near $\lambda = 0$, we get from Eq.(19)

$$F^{singular}(J_1^{(r)}, J_2^{(r)}, J_3^{(r)}, J_4, \lambda^{(r)}) \approx (1/2)\, F^{singular}(J_1^{(r+1)}, J_2^{(r+1)}, J_3^{(r+1)}, J_4, \lambda^{(r+1)}) . \quad (23)$$

It can be shown that Eqs. (22b-d) imply that $J_2^{(r)}/J_1^{(r)}$ and $J_3^{(r)}/J_1^{(r)}$ tend to finite asymptotic values ($2^{1/3} + 2^{-1/3}$) and $2^{-1/3}$ geometrically with large r. Hence for large enough r the

eqs. (22a-d) have the form

$$\lambda^{(r+1)} \approx 2\,\lambda^{(r)} , \tag{22a}$$

$$J_1^{(r+1)} \approx 2^{-1/3}\, J_1^{(r)} , \tag{22b}$$

$$J_2^{(r+1)} \approx 2^{-1/3}\, J_2^{(r)} , \tag{22c}$$

$$J_3^{(r+1)} \approx 2^{-1/3}\, J_3^{(r)} . \tag{22d}$$

Now, since the variables $J_2^{(r)}$ and $J_3^{(r)}$ are asymptotically proportional to $J_1^{(r)}$ for large r , these variables are unnecessary for our discussion . Any one of the variables $J_1^{(r)}$, $J_2^{(r)}$, $J_3^{(r)}$ is adequate for the discussion of the critical properties of our model. These variables provide a relevant scale for our problem. We assume that $F^{Singular}(J_1^{(r)}, J_2^{(r)}, J_3^{(r)}, \lambda^{(r)})$ $\approx A(\lambda^{(r)} J_4 / J_1^{(r)})^{d/2}$, where A is some constant. Substituting this in Eq.(23) and with the help of Eqs.(24a-b) we find that d=3/2, which is the promised result.

VI : THE SPHERICAL MODEL

The spherical model was first proposed by Kac [28] in 1947, and later solved exactly by Montroll [29]. We give here a brief review of its critical properties for arbitrary space dimensionality d. A more detailed and exhaustive review is given by Joyce [30]. No new results are presented in this section. Our purpose here is only to illustrate by an explicit example how the critical exponents depend piecewise continuously on the space dimensionality d. Also, these calculations constitute an important argument in favor of our definition of dimensionality, since the critical exponents agree with the expressions derived in literature using formal arguments only. Our treatment here is brief. For a more complete discussion, the reader is referred to the review article by Joyce.

The spherical model assigns a continuous spin χ_i $(-\infty < \chi_i < +\infty)$ to each site i of a d-dimensional lattice. The Hamiltonian of the system is given by

$$H = +(J/2) \sum_{(ij)} (\chi_i - \chi_j)^2 \quad - h \sum_i \chi_i \quad . \tag{25}$$

Here J is the ferromagnetic coupling constant between the spins. h is an external magnetic field. The summation over (i,j) runs over all nearest neighbor pairs. The spins are

subjected to the constraint

$$\sum_i \chi_i^2 = N \ , \tag{26}$$

where N is the total number of sites on the lattice. The partition function of the system is given by

$$Z(\beta,h) = \prod_{i=1}^{N} \left(\int_{-\infty}^{+\infty} d\chi_i \right) \exp(-\beta H) \ \delta\left(\sum_i \chi_i^2 - N\right) \ , \tag{27}$$

where β is the inverse temperature. The partition function may be evaluated easily using Laplace transforms. We write

$$\delta\left(\sum_i \chi_i^2 - N\right) = \int_{-i\infty}^{+i\infty} \exp\left[-\lambda \beta J \left(\sum_i \chi_i^2 - N\right)/2\right] \beta J \, d\lambda/(4\pi i) \ . \tag{28}$$

We substitute this representation of the delta function into Eq.(27). The integrations over χ_i are now Gaussian , and may be done easily to give

$$Z(\beta,h) = \left(\frac{\beta J}{4\pi i}\right) \int_{-i\infty}^{+i\infty} d\lambda \exp[\beta\lambda N J/2] \ \Omega(\beta,\lambda) \exp[N h^2 \beta/2\lambda J]. \tag{29}$$

with

$$\Omega(\beta,\lambda) = \prod_i \left(\int_{-\infty}^{+\infty} d\chi_i \right) \exp\left[-\beta \sum_{(ij)} J(\chi_i - \chi_j)^2/2 - (\lambda \beta J/2)\left(\sum_i \chi_i^2\right)\right]$$
$$= (2\pi/\beta J)^{N/2} \prod_i (\omega_i^2 + \lambda)^{-1/2} \ . \tag{30}$$

Here ω_i^2 are the normal mode frequencies of the Hamiltonian H. The integral in Eq.(29) may be evaluated using the method of steepest descent. We get , retaining only terms linear in N,

$$\ln Z(\beta,h) = \ln \Omega(\beta,\lambda_0) + N \beta h^2/(2\lambda_0 J) + N \beta \lambda_0 J/2 \ , \tag{31}$$

where λ_0 is the point where the right hand side of Eq.(31) attains its maximum value and thus is determined by the equation

$$(1/N)\sum_i (\omega_i^2+\lambda_o)^{-1} = \beta J - \beta h^2/(\lambda_o^2 J) \quad . \tag{32}$$

First consider the case h=0. Then the equation determining λ_o is

$$\int_o^\infty D(\omega^2)d\omega^2\ (\omega^2+\lambda_o)^{-1} = \beta J \quad . \tag{33}$$

Here $D(\omega^2)$ is the spectral density function. $D(\omega^2)d\omega^2$ is the fractional number of modes in the frequency range ω^2 and $\omega^2+d\omega^2$. Using our definition of effective dimensionality

$$D(\omega^2) = K\,\omega^{d-2} \quad , \text{ for small } \omega \ , \tag{34}$$

where K is some constant of proportionality. Three different cases arise.

Case I : $d<2$. The integral on the left hand side of Eq.(33) diverges for small λ_o as $\lambda_o^{\frac{d-2}{2}}$. Hence for large β,

$$\lambda_o \approx \beta^{\frac{2}{d-2}} \tag{35}$$

For any finite β, λ_o is finite and a smooth function of β. Consequently the free energy is a smooth function of β, and no phase transition occurs at non-zero temperatures. Since the critical temperature is zero , the critical exponents cannot be defined unambigously in this case. We note , however, that as β tends to infinity, the magnetic susceptibility of the model is given by

$$\chi = (1/\beta N)\frac{\partial^2}{\partial h^2}\ln Z(\beta,h)\Big|_{h=o} = (1/\lambda_o J) \approx \beta^{\frac{2}{2-d}} \quad . \tag{36}$$

The energy is obtained by differentiating $\ln Z(\beta,h)$ with respect to β and from Eqs.(31) and (33); it is easily seen

that the energy per site is given by

$$E = 1/2\beta) - \lambda_o J/2 = (1/2)\,(1/\beta - 1/\chi)\ . \qquad (37)$$

This relation between the internal energy per site and the zero field susceptibility is valid for higher dimensions also for $\beta < \beta_c$. The specific heat per site for low temperatures is given by

$$C_v(\beta) = (\beta^2/N)\frac{\partial^2}{\partial\beta^2} \ln Z(\beta, h=0) \approx 1/2 - K\beta^{\frac{d}{d-2}}\ , \qquad (38)$$

where K is some constant of proportionality, and we have ignored higher order singular terms in β.

Case II : $2 < d < 4$. In this case, the integral on the left hand side of Eq.(33) converges for $\lambda_o = 0$. Define β_c by the equation

$$\int_o^\infty D(\omega^2)\, d\omega^2/\omega^2 = \beta_c J\ . \qquad (39)$$

For $\beta > \beta_c$, Eq.(33) ceases to be valid. The phenomenon is analogous to the onset of condensation in an ideal Bose gas. λ_o becomes exactly zero and q_o, the normal mode coordinate corresponding to the zero frequency mode, becomes very large, of order $\sqrt{N}$. This is the onset of spontaneous magnetization in this model.

If $\beta = \beta_c(1-\varepsilon)$, where ε is a small negative quantity, we get

$$q_o^2 = -N \varepsilon \beta_c J \ . \qquad (40)$$

But q_o^2/N is the square of the spontaneous magnetization in the model. Hence we get for the critical exponent β, which measures the rate at which the spontaneous magnetization increases as a function of ε,

$$\beta = 1/2 \ . \qquad (41)$$

This critical exponent β should not be confused with the inverse temperature β used everywhere else in this discussion. Also, for $\beta > \beta_c$, $\lambda_o = 0$, and the energy satisfies the equation

$$E(\beta > \beta_c \ , h=0) = 1/(2\beta) \ . \qquad (42)$$

Thus the specific heat below the critical temperature is a constant, and the corresponding critical exponent ($C_v \sim |\varepsilon|^{-\alpha'}$) is

$$\alpha' = 0. \qquad (43)$$

Below the critical temperature, the magnetization is a nonanalytic function of the external field h. Hence the susceptibility below the critical temperature is infinite, and the critical exponent γ', which specifies the divergence of susceptibility below the critical temperature ($\chi \sim |\varepsilon|^{-\gamma'}$), is undefined.

To discuss the critical properties of the spherical model in the presence of an external field h, it is convenient to work with a constant magnetization ensemble,

instead of the constant external field. For a fixed magnetization m, the Eqs.(31) and (32) may be easily seen to yield ,except for irrelevant additive constants

$$(1/N)\ \ell n\ Z(\beta, h, m) = -\tfrac{1}{2}\int_0^\infty \frac{D(\omega^2)\,\omega^2}{\omega^2+\lambda_0}\,d\omega^2 + \beta h m - \tfrac{1}{2}\ell n(\beta J) - \tfrac{1}{2}\int_0^\infty D(\omega^2)\,d\omega^2\,\ell n(\omega^2+\lambda_0), \tag{44}$$

where λ_0 is determined by the condition

$$(1/\beta J)\int_0^\infty D(\omega^2)\frac{1}{\omega^2+\lambda_0}\,d\omega^2 + m^2 = 1\ . \tag{45}$$

Different terms in Eq.(44) are easy to identify. The first term is the ferromagnetic interaction energy of the spins. The second term gives the interaction energy with the external field. The third and the fourth terms give the entropy contribution due to the normal modes. Eq.(45) is essentially the same as Eq.(33) with the contribution m^2 due to the zero frequency mode explicitly written out.

To determine the equilibrium value of $m(\beta, h)$, we have to maximize $\ell n\ Z(\beta, h, m)$ with respect to m. Setting its partial derivative with respect to m equal to zero , we get

$$\left[\tfrac{1}{2}\int_0^\infty d\omega^2 D(\omega^2)\frac{\omega^2}{(\omega^2+\lambda_0)^2}\right]\frac{\partial\lambda_0}{\partial m} + \beta h - \tfrac{1}{2}\left[\int_0^\infty D(\omega^2)\frac{1}{\omega^2+\lambda_0}d\omega^2\right]\frac{\partial\lambda_0}{\partial m} = 0\ . \tag{46}$$

But from Eq.(45)

$$\left[\frac{\partial\lambda_0}{\partial m}\right]\left[-\frac{1}{\beta J}\int_0^\infty D(\omega^2)\frac{1}{(\omega^2+\lambda_0)^2}d\omega^2\right] + 2m = 0\ . \tag{47}$$

Substituting in Eq.(46) we get after some simple algebra

$$m\lambda_0 J = h\ . \tag{48}$$

Now we recall that $D(\omega^2)$ is proportional to ω^{d-2} for small ω . Hence we may write for small λ_0

$$\int_c^\infty D(\omega^2)\frac{1}{\omega^2+\lambda_0}\,d\omega^2 \approx \beta_c J - K_1 \lambda_0^{\frac{d-2}{2}} - K_2 \lambda_0 + \text{higher order terms in } \lambda_0 , \quad (49)$$

where K_1 and K_2 are some constants dependent on the lattice. If $d < 4$, then the K_2 term is of higher order than the K_1 term and may be ignored. Substituting the value of λ_0 from Eq.(48) into Eq.(45), and making use of the approximation of Eq.(49) , we get to the lowest power in h

$$\beta J(1 - m^2) \approx \beta_c J - K_1 (h/mJ)^{\frac{d-2}{2}} . \quad (50)$$

From this equation of state, the critical exponents are easily determined. Consider $\beta = \beta_c$. Then the critical exponent δ , which determines the magnetization as a function of the external field at the critical point ($h \sim m^\delta$), is easily seen to be

$$\delta = (d+2)/(d-2) , \text{ for } 2<d<4. \quad (51)$$

Also, if $\beta > \beta_c$, the magnetization m is seen to be a nonanlytical function of h, and hence the susceptibility exponent γ' ($\chi \sim |\beta-\beta_c|^{-\gamma'}$, for $\beta > \beta_c$) is undefined.

If $\beta < \beta_c$, then for small external field h , m is small and may be neglected in the left hand side of Eq.(50) . This gives

$$\chi = m/h \approx (\beta_c - \beta)^{\frac{2}{2-d}} . \quad (52)$$

Hence we get the critical exponent

$$\gamma = 2/(d-2) \ . \qquad (53)$$

Also, from Eqs.(33) and (49) we see that for $\beta < \beta_c$

$$\lambda_0 \approx (\beta_c - \beta)^{\frac{2}{d-2}} \ . \qquad (54)$$

But from Eq.(37) we know that the singular behavior of λ_0 is the same as the singular behavior of the energy. Hence we see that the specific heat exponent α ($C_v \sim (\beta_c - \beta)^{-\alpha}$ for $\beta < \beta_c$) is given by

$$\alpha = (d-4)/(d-2) \ . \qquad (55)$$

Case III : $d > 4$. The treatment of this case is identical to the previous one. The only difference is that for $d > 4$, in Eq.(49) , the K_2 term dominates over the K_1 term . The Eq.(50) is modified to

$$\beta J(1 - m^2) \approx \beta_c J - K_2 h/m \ . \qquad (56)$$

The critical exponents in this case are derived similarly. We get

$$\alpha' = 0. \qquad (57)$$

$$\gamma' = \text{undefined} \ . \qquad (58)$$

$$\delta = 3. \qquad (59)$$

$$\gamma = 1. \qquad (60)$$

$$\alpha = 0. \qquad (61)$$

$$\beta = 1/2. \qquad (62)$$

Hence for $d>4$, the critical exponents are independent of dimensionality and have the same values as for $d=4$.

All the critical exponents are seen to satisfy the scaling relations

$$\delta = 1 + \gamma/\beta \, . \tag{63}$$

$$\alpha + 2\beta + \gamma = 2 \, . \tag{64}$$

In the literature [31] , many other scaling relations are discussed. They however involve additional exponents like ν or η etc. . These exponents depend on the rate of decay of the correlation function near the critical point, and are difficult to define because of the spatial inhomogeneity of the lattices studied here. Scaling relations involving these exponents are not included here. We shall return to this point in the next section.

VII : THE CLASSICAL XY MODEL

In the classical XY model , a spin direction θ_i, $0 \leq \theta_i \leq 2\pi$, is assigned to each site i of the lattice. The Hamiltonian of the system is given by

$$H = -J \sum_{(ij)} \cos(\theta_i - \theta_j) - h \sum_i \cos\theta_i , \tag{65}$$

where the summation over (ij) extends over all pairs of nearest neighbor sites. The corresponding partition function is given by

$$Z = \prod_i \left(\int_0^{2\pi} \frac{d\theta_i}{2\pi} \right) \exp(-\beta H) . \tag{66}$$

First consider the case of zero external field h. We write

$$\exp[\beta J \cos(\theta_i - \theta_j)] = \sum_{n_{ij}=-\infty}^{+\infty} I_{n_{ij}}(\beta J) \exp[i n_{ij} (\theta_i - \theta_j)], \tag{67}$$

where $I_m(x)$ is the modified Bessel function of x of order m, and express Z as a summation over all possible values of $\{n_{ij}\}$. With each term of this summation we associate an arrow configuration on the bonds of the lattice. The arrow configuration has n_{ij} arrows going from site i to site j, for all nearest neighbor sites and with the convention $n_{ij} = -n_{ji}$. Thus the partition function is expressed as a sum over all possible arrow configurations. The weight of a bond with m arrows is $I_m(\beta J)$. The integrations over $\{\theta_i\}$ are trivial and show that only those configurations of arrows contribute to the partition function sum in which the total

number of arrows going into any site is zero.

Equivalently we may assign a weight $T(m_1, m_2, m_3)$ to a vertex with m_1, m_2, m_3 arrows going into it from its three nearest neighbors. If $m_1 + m_2 + m_3 \neq 0$, we set the corresponding vertex weight $T(m_1, m_2, m_3) = 0$.

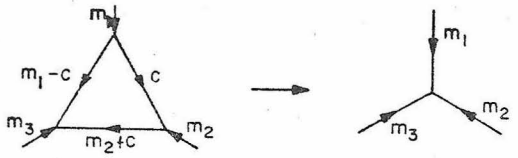


FIG. 9. The renormalization transformation for the XY model on the truncated 3-simplex lattice. The three vertices in the left figure are replaced by a single vertex.

The renormalization procedure for the truncated 3-simplex lattice consists of replacing a group of three neighboring vertices by a single vertex and is illustrated in Fig 9. If $T^{(r)}(m_1, m_2, m_3)$ denotes the vertex weight after r iterations, the renormalization equations are given by

$$T^{(r+1)}(m_1, m_2, m_3) = \sum_{c=-\infty}^{+\infty} T^{(r)}(m_1, c-m_1, -c) T^{(r)}(m_3, m_1-c, c+m_2) T^{(r)}(m_2, c, -c-m_2). \tag{68}$$

The starting values of vertex weights are

$$T^{(0)}(m_1, m_2, -m_1-m_2) = [I_{m_1}(\beta J) I_{m_2}(\beta J) I_{-m_1-m_2}(\beta J)]^{1/2}. \tag{69}$$

The free energy per site is given by

$$f(\beta)=-\frac{1}{\beta}\lim_{r\to\infty} 3^{-r}\ \ln T^{(r)}(0,0,0). \tag{70}$$

It is easy to verify that Eqs. (68) have only one attractive fixed point given by

$$T^{(r)}(m_1,m_2,m_3)/T^{(r)}(0,0,0)=\delta_{m_1,0}\delta_{m_2,0}\delta_{m_3,0}.$$

This corresponds to spin directions at large distances being uncorrelated, and hence to the absence of spontaneous magnetization in this system. If the temperature is very low, $\beta J>>(m_1^2+m_2^2+m_3^2)$, we have

$$T^{(0)}(m_1,m_2,-m_1-m_2)$$
$$\approx A^{(0)}\exp[-\{m_1^2+m_2^2+(-m_1-m_2)^2\}/4\beta J]. \tag{71}$$

If βJ is very large, we may replace the summation over c in Eq.(68) by an integration. Substituting the values of the weights $T^{(0)}(m_1,m_2,m_3)$ from Eq. (71) we get

$$T^{(1)}(m_1,m_2,-m_1-m_2)$$
$$\approx A^{(1)}\exp[-5\{m_1^2+m_2^2+(-m_1-m_2)^2\}/12\beta J], \tag{71a}$$

where $A^{(0)}$ and $A^{(1)}$ are some constants. This shows that the renormalization equation for the temperature is

$$\beta'=3\beta/5. \tag{72}$$

Now let us introduce a small external field h, $\beta h<<1$. It is easy to see that the vertex weights $T(m_1,m_2,m_3)$ are no longer zero if $m_1+m_2+m_3\neq 0$. To first order in βh, and for $\beta J>>(m_1^2+m_2^2+m_3^2)$ the other nonzero vertex weights are

$$T^{(0)}(m_1,m_2,m_3)=\beta h A^{(0)}\exp[-\{m_1^2+m_2^2+m_3^2\}/4\beta J],$$
$$\text{for } m_1+m_2+m_3=\pm 1. \tag{73}$$

After one renormalization , using Eq.(68) these are easily seen to transform to

$$T^{(1)}(m_1,m_2,m_3)=3\beta h A^{(1)} \exp[-5\{m_1^2+m_2^2+m_3^2\}/12\beta J] ,$$
$$\text{for } m_1+m_2+m_3=\pm 1. \tag{74}$$

Thus we see that to the lowest order in βh, the external field h is transformed according to the renormalization equation

$$\beta' h' = 3\beta h. \tag{75}$$

Using Eqs. (72) and (75) , it is easy to determine the behavior of the susceptibility as a function of temperature. Let $g(\beta,h)$ be the singular part of the logarithm of the partition function per spin. By the renormalization transformation

$$g(\beta,h)=(1/3)\ g(3\beta/5,5h), \tag{76}$$

and the susceptibility

$$\chi(\beta)= -\frac{1}{\beta}\frac{\partial^2}{\partial h^2} g(\beta,h)\Big|_{h=0} = -\frac{5}{\beta'}\frac{\partial^2}{\partial h'^2} g(\beta',h')\Big|_{h'=0}$$
$$=5\chi(3\beta/5). \tag{77}$$

Hence if $\chi(\beta)\sim\beta^{-\bar{\gamma}}$ we get

$$\bar{\gamma} = \ln 5/(\ln 5-\ln 3). \tag{78}$$

Similar analysis of the truncated n-simplex lattice for arbitrary n shows that in general , for $d<2$

$$\bar{\gamma} = 2/(2-d). \tag{79}$$

The specific heat tends to the simple harmonic oscillator value $\frac{1}{2}K_B$ as the temperature tends to zero.

These results are easily extended to the case when the spin at each site is a p-dimensional vector $\vec{S}$ of unit magnitude. Here p is an arbitrary integer greater than or equal to 2. p=2 corresponds to the XY model. p=1 corresponds to the Ising model which differs from the rest in being a discrete rather than a continuum model and is discussed in the next section.

The recursion equations for the coupling constants βJ and βh for the p-vector model (p>2) are still given by Eqs.(72) and (75). For low enough temperature, the angle between nearest neighbor spins is small and interaction between them may be replaced by a harmonic spring coupling. Eq.(72) just shows how the harmonic spring coupling constants are transformed for the truncated 3-simplex lattice under the renormalization transformation. Also, Eq.(75) follows from the fact that the nearest neighbor spins are very closely aligned at low temperatures. Consider a renormalization transformation under which three spins on a first order triangle α; $\vec{S}_{\alpha 1}$, $\vec{S}_{\alpha 2}$, $\vec{S}_{\alpha 3}$ are replaced by a block spin $\vec{S}_{\alpha}$. The effective coupling of these spins to a small external field h is given by $-\beta\vec{h}.(\vec{S}_{\alpha 1}+\vec{S}_{\alpha 2}+\vec{S}_{\alpha 3})$.

This is approximately equal to $-3\beta\vec{h}.\vec{S}_{\alpha}$ since $\vec{S}_{\alpha} \approx \vec{S}_{\alpha i}$ for most configurations. This gives us the renormalization equation (75).

Since the renormalization equations are independent of p, we conclude that the critical behavior of the model is also independent of p, for p>2, for the truncated 3-simplex lattice (in general for lattices with d<2). This conclusion is of some interest because it is known to be false for d>2, and series expansions for critical exponents in powers of (1/p) exist in literature [32]. In particular , the case $p \longrightarrow \infty$ corresponds to the spherical model [33] discussed in the previous section.

The exponent $\bar{\gamma}$ in Eq.(79) should not be identified with the critical exponent γ which appears in the scaling equations and specifies the divergence of susceptibility as a function of temperature slightly away from the critical point. The reason is the arbitrariness in the definition of critical exponents when the critical temperature is zero. The procedure of determining the critical exponents in terms of the divergence of correlation length is of doubtful validity here because the lattice is not translationally invariant and the "correlation length" is a function of position. Different definitions of "averaged correlation length" may well give rise to difference dependence on temperature. In general, it is difficult to find a useful

definition of correlation length for the spatially inhomogenous and highly anisotropic lattices studied here. Consequently the critical indices ν and η are undefined even if the transition temperature is finite. (To define them in terms of scaling relations would be begging the question.) The critical exponents like α, β, γ or δ etc. [34], which may be defined by differentiation of thermodynamic quantities, are however well defined for nonzero transition temperatures.

VIII : THE FORTUIN-KASTELEYN CLUSTER MODEL

The cluster model was introduced by Fortuin and Kasteleyn [35-37]. It is defined in terms of a parameter K and includes as special cases the percolation model ($K=1$), the Ising model ($K=2$), resistive networks ($K=0$), and the n-state Potts model($K=n$) [38].

The partition function of the cluster model for any given graph is given by

$$Z(p,K)=\sum_{C} p^{r(C)}(1-p)^{N-r(C)} \; K^{\gamma(C)},$$

where N is the total number of bonds in the graph. The summation extends over all possible configurations C of "occupied" or "unoccupied" states of bonds on the lattice. $r(C)$ is the number of occupied bonds in the configuration C and $\gamma(C)$ is the number of distinct clusters in configuration C. Fortuin and Kasteleyn have called this the random cluster model. However, the model is completely specified by a Hamiltonian which has a term proportional to the total number of occupied bonds and a term proportional to the total number of clusters . It is thus no more random than any other statistical mechanical system, and the adjective "random" is unnecessary.

Due to its very general nature, the cluster model is of much interest in statistical physics. However, for arbitrary values of K, the model has not been solved even in two dimensions. We sketch below the renormalization group treatment of this model for the truncated tetrahedron lattice. It is shown that the model does not show any phase transition for any values of K and p such that $K>0$, and $0 \leqslant p<1$.

We define the restricted partition functions $Z^{(r)}(a|b|c)$, $Z^{(r)}(a|bc)$, $Z^{(r)}(b|ac)$, $Z^{(r)}(c|ab)$, and $Z^{(r)}(abc)$. Here $Z^{(r)}(a|b|c)$ is the partition function of the r^{th} order triangle, whose corner vertices are a,b,c and the summation corresponds to all configurations of edges within the triangle subject to the constraint that no sequence of occupied bonds within the triangle connects any two of the vertices a,b,c. $Z^{(r)}(abc)$ is the restricted partition function when a,b,c are connected together by bonds lying within the r^{th} order triangle. $Z(a|bc)$ etc. are defined similarly. By symmetry between the corner vertices a,b and c, we have

$$Z^{(r)}(a|bc) = Z^{(r)}(b|ac) = Z^{(r)}(c|ab) = Z_1^{(r)}, \quad \text{(say)} \qquad (8.1a)$$

and we write

$$Z^{(r)}(a|b|c) = Z_1^{(r)}, \tag{81b}$$

$$Z^{(r)}(abc) = Z_3^{(r)}. \tag{81c}$$

It is quite straightforward , though tedious , to write down the expressions for $Z_1^{(r+1)}$, $Z_2^{(r+1)}$, $Z_3^{(r+1)}$ in terms of $Z_1^{(r)}$, $Z_2^{(r)}$, and $Z_3^{(r)}$ by summing over the 2^3 possible states of the three bonds that connect the r^{th} order triangles to form a $(r+1)^{th}$ order triangle and grouping together terms that correspond to the same connectivity structure of the $(r+1)^{th}$ order triangle. The result is

$$\begin{aligned} Z_1^{(r+1)} = {} & q^3(Z_1+3Z_2+Z_3)^3 \\ & +3pq^2\kappa^{-1}(Z_1+3Z_2+Z_3)(Z_1+2Z_2)(Z_1+4Z_2+2Z_3) \\ & +3p^2q\kappa^{-2}\{(Z_1+2Z_2)^3+3(Z_1+2Z_2)^2(Z_2+Z_3)+Z_1(Z_2+Z_3)^2\} \\ & +p^3\kappa^{-3}\{\kappa(3Z_3Z_1^2+Z_2^3)+14Z_2^3+12Z_1Z_2Z_3+24Z_2^2Z_1+3Z_1^2Z_3+9Z_1^2Z_2+Z_1^3\}, \end{aligned} \tag{82a}$$

$$Z_2^{(r+1)} = q^2p\kappa^{-1}(Z_1+3Z_2+Z_3)(Z_2+Z_3)^2+p^2q\kappa^{-2}(Z_2+Z_3)^2(2Z_1+7Z_2), \tag{82b}$$

$$Z_3^{(r+1)} = 3p^2q\kappa^{-2}(Z_2+Z_3)^2Z_3+p^3\kappa^{-3}(\kappa Z_3^3+6Z_2Z_3^2+3Z_2^2Z_3), \tag{82c}$$

where we have put $q=1-p$, and $Z_i^{(r)}=Z_i$, $i=1,2,3$. In Appendix B, we have listed the configurations of r^{th} order triangles that form an (r+1)th order triangle with all its corner vertices belonging to the same cluster. The sum of the weights of these configurations appears on the right hand side of Eq.(82c). Eqs.(82a) and (82b) are written down similarly.

If $q > 0$, analysis of these equations shows that there exists only one fixed point , which is attractive and corresponds to $Z_2^{(r)}/Z_1^{(r)} = Z_3^{(r)}/Z_1^{(r)} = 0$. This implies the absence of phase transitions at any finite temperature. For small q and small r, $Z_3^{(r)}$ is much larger than $Z_1^{(r)}$ or $Z_2^{(r)}$. If we renormalize the $Z_i^{(r)}$ after each iteration so that $Z_1^{(r)} + 3Z_2^{(r)} + Z_3^{(r)} = 1$ always, we get to the lowest order in q

$$Z_1^{(r)} = K^2 q^3, \tag{83a}$$

$$Z_2^{(r)} = K q^2 r, \tag{83b}$$

$$Z_3^{(r)} = 1 - 3q^2 K r. \tag{83c}$$

Thus for very small r, $Z_2^{(r)}$ increases linearly with r. This, however , is not true for larger values of r, when $Z_2^{(r)}$ becomes comparable to q, and is not of order q^2. Let us assume that the value of $Z_2^{(r)}$ is $\varepsilon^{(r)}$ with $1 >> \varepsilon^{(r)} >> q^2 K$. Then it is easy to see from eq.(82a) and the condition $Z_1^{(r)} + 3Z_2^{(r)} + Z_3^{(r)} = 1$, that to second order in $\varepsilon^{(r)}$ the values of $Z_i^{(r)}$ are given by

$$Z_1^{(r)} = 3\varepsilon^{(r)2}, \tag{84a}$$

$$Z_2^{(r)} = \varepsilon^{(r)}, \tag{84b}$$

$$Z_3^{(r)} = 1 - 3\varepsilon^{(r)} - 3\varepsilon^{(r)2}. \tag{84c}$$

Substituting these values in the recursion equations (82) we can determine $\varepsilon^{(r+1)}$ up to second order in q and $\varepsilon^{(r)}$. We get

$$\varepsilon^{(r+1)} = \varepsilon^{(r)} + 4\varepsilon^{(r)2}K^{-1} + 4q\varepsilon^{(r)} + Kq^2. \tag{85}$$

This shows that

$$\varepsilon^{(r+1)} - \varepsilon^{(r)} \approx 4(\varepsilon^{(r)} + qK/2)^2/K. \tag{86}$$

Since $\varepsilon^{(r)}$ is small compared to one, its value changes slowly with r and we may approximate the difference equation (86) by the corresponding differential equation

$$\frac{d\varepsilon^{(r)}}{dr} \approx 4(\varepsilon^{(r)} + qK/2)^2/K. \tag{87}$$

This equation has the solution

$$(\varepsilon^{(r)} + \tfrac{qK}{2})^{-1} - (\varepsilon^{(0)} + \tfrac{qK}{2})^{-1} \approx 4r/K \tag{88}$$

This equation determines $\varepsilon^{(r)}$ as a function of r. Let us determine the value of r when $\varepsilon^{(r)}$ becomes comparable to 1. Call this r_c. We may put $\varepsilon^{(0)}=0$, $\varepsilon^{(r_c)}=0.2$ (typically). For very small q we get the approximate equation

$$r_c = 1/(2q) - AK. \tag{89}$$

Here A is some constant which depends on the precise value of cutoff, and thus perhaps depends weakly on K.

Now, the mean size of a cluster is obviously given by $B3^{r_c}$, where B is some finite constant dependent on the cutoff. We have thus deduced that for small $q<<1/K$, the mean size of a cluster is approximately given by $B(K)3^{\frac{1}{2q}}$. This result has already been obtained by Nelson and Fisher for the particular case of the Ising model. The mean size of a cluster in the Fortuin-Kasteleyn cluster model

corresponds to the susceptibility of the Ising model [39]. We need only note the correspondence $K=2$ and $q=\exp(-2\beta J)$, to specialize our result to this particular case.

Other lattices with $1<d<2$ give very similar results. In each case the mean size of a cluster varies as the exponential of the exponential of inverse temperature. To appreciate how close these systems are to phase transitions, one need only observe that the susceptibility of the Ising model on the truncated tetrahedron lattice is of the order of 200 when $\beta J=1$. When $\beta J=3$, the logarithm of the susceptibility is approximately 220. If these lattices were experimentally accessible, an experimentalist would certainly conclude that the system shows spontaneous magnetization at low temperatures, since it would be quite impossible to eliminate external magnetic fields so completely. Or , for that matter, to find samples sufficiently large so that the volume of the experimental sample is comparable to the correlation volume.

IX : SELF-AVOIDING RANDOM WALKS

Self-avoiding random walks were originally proposed as a model of polymers , to study the effect of excluded volume [40]. The properties of these walks are connected with some properties of the Ising model [41]. The study of the configurational problems encountered in this problem may be expected to shed some light on the more general problem of second order phase transitions . The problem has been attacked using a variety of numerical and analytical techniques [42-44] , but the number of exact results known is small . It has resisted a complete solution in the physically interesting case of three dimensions , or even in the considerably simpler case of two dimensions.

It is thus of some interest to study the problem for some psuedo-lattices , where the exact solution may be worked out and its properties analysed in detail. The analysis in this section differs from the previous two mainly in that for the self avoiding walk problems, the recursion equations have nontrivial fixed points, even for lattices with effective dimensionality less than two. The system shows a phase transition in the sense that the generating functions of the random walk become singular as a function of their argument. We can determine the critical

exponents using standard renormalization group techniques.

The recursion equations are coupled algebraic equations and their derivation and analysis is quite straightforward. In the parameter space of the coupling constants , we observe the phenomenon of the point specifying the effective interaction approaching the fixed point of the renormalization transformation initially. Eventually the point escapes away from the fixed point after a large number of iterations unless the starting system was exactly critical. Linearizing the recursion equations about the fixed point, we determine the critical exponents from the eigenvalues of the linearized renormalization transformation matrix.

A self avoiding walk on a lattice is a random walk with the constraint that no lattice point is visited more than once. We associate a weight factor x with each step of the walk and define the generating functions

$$C(x) = \lim_{N\to\infty} (1/N)\sum_{n=0}^{\infty} C_n(N)\, x^n \qquad (90)$$

$$P(x) = \lim_{N\to\infty} (1/N)\sum_{n=2}^{\infty} P_n(N)\, x^n \qquad (91)$$

Here $C_n(N)$ is the total number of distinct self avoiding random walks of n steps on a large lattice consisting of N points. $P_n(N)$ is the number of distinct closed simple polygons of perimeter n on the lattice . The

random walk may start from any point on the lattice. For large N , the numbers $C_n(N)$ and $P_n(N)$ are asymptotically proportional to N , and the limit exists. For regular lattices, where all the lattice points are equivalent , this limiting procedure is unnecessary because the number of self avoiding walks of length n is independent of the vertex from which the walk starts (so long as the starting vertex is not too close to the boundary of the lattice) . This is not the case for the spatially inhomogenous lattice studied here and the averaging over all possible positions of the starting point is necessary. We define

$$\overline{P_n} = \lim_{N\to\infty} P_n(N)/N \ , \tag{92}$$

$$\overline{C_n} = \lim_{N\to\infty} C_n(N)/N \ . \tag{93}$$

We know that for large n, $\overline{P_n}$ and $\overline{C_n}$ increase geometrically with n. Let us assume that for large n

$$\overline{P_n} \sim K_1 \mu^n n^{\alpha-3} \ , \tag{94}$$

$$\overline{C_n} \sim K_2 \mu^n n^{\gamma-1} \ , \tag{95}$$

where K_1 and K_2 are some coefficients of proportionality. In general , we represent a constant of proportionality by K, with or without subscripts . Its numerical value is not necessarily the same in different equations. μ is called the connectivity constant of the lattice , and α and γ are critical indices for the random walk. Substituting the asymptotic behavior of $\overline{C_n}$ and $\overline{P_n}$ into Eqs. (90) and (91) we

find that as x tends to $1/\mu$ from below, the asymptotic behavior of C(x) and P(x) is given by

$$C(x) \approx K_2 (1-x\mu)^{-\gamma} + \text{less singular terms} , \qquad (96)$$

$$P(x) \approx K_1 (1-x\mu)^{2-\alpha} + \text{less singular terms} . \qquad (97)$$

The average number of self avoiding walks per site that return to the origin (polygonal closures) after exactly n steps is given by $2n\bar{P}_n$. We also define the generating function for the mean squared end to end distance by

$$R(x) = \lim_{N\to\infty} (1/N) \sum_{L} [R(L)]^2 \, x^{n(L)} , \qquad (98)$$

where R(L) is the end to end distance for the random walk L with total number of steps given by n(L) . The summation extends over all possible self avoiding random walks L on a large lattice of size N . We define the critical exponent ν by the relation

$$\langle R_n^2 \rangle \approx K \, n^{2\nu} , \quad \text{for large n} , \qquad (99)$$

where $\langle R_n^2 \rangle$ is the mean squared end to end distance for n-step self avoiding random walks , all walks being weighted equally. Since the number of such walks increases as $n^{\gamma-1}\mu^n$ (Eq. (95)), we find that the asymptotic behavior of R(x) as $x\mu \to 1$ from below , is given by

$$R(x) \sim K(1-x\mu)^{-\gamma-2\nu} + \text{less singular terms} . \qquad (100)$$

We use the renormalization group techniques to determine the constants μ, α, γ and ν for the truncated tetrahedron lattice by determining the singular behavior of the generating functions C(x) , P(x) , and R(x). We shall show that for the truncated tetrahedron lattice

$$\mu = 1.6180 \quad , \quad \alpha = 0.7342 \quad , \quad \gamma = 1.3752 \quad , \quad \nu = 0.7986 \quad . \tag{101}$$

We now derive these connectivity constant and critical indices. The generating functions C(x) , P(x) and R(x) are weighted sums over self avoiding random walks . The weight of a walk of length n is x^n . For R(x) , there is an additional multiplicative weight factor depending on the end to end distance of the walk (Eq. (98)). Instead of assigning a weight x to each step of the walk , we may equivalently assign a weight x to each vertex the walk passes through, and a weight $\sqrt{x}$ to each of the two vertices that are the end points of the walk . Then , for example , P(x) is is the sum over all possible configurations with a single loop .

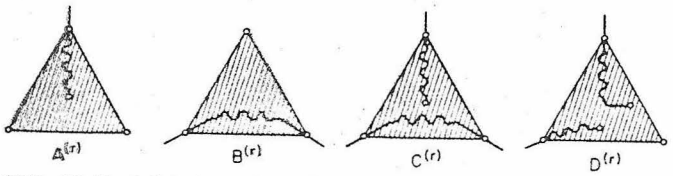


FIG. 10. Restricted partition functions for an rth order triangle. The shaded triangles denote rth order triangles, of which only the corner vertices and the end points of the self-avoiding walks are shown.

The renormalization transformation consists of summing over all internal configurations of rth order triangles, as was done for the Fortuin-Kasteleyn model in Section VIII. We define the r^{th} order weights as shown in Figure 10. Here $A^{(r)}$ is the weight of an r^{th} order triangle with one line going in. The end point of the line may be any of the vertices inside the r^{th} order triangle. We sum over all possible configurations of the r^{th} order triangle consistent with the constraint that one of the end points of the walk lies inside it . Similarly $B^{(r)}$ is the weight of an r^{th} order triangle in which a line goes into the triangle from one of the corner vertices and comes out of another. (The lines are undirected. We use the terms going in and coming out rather loosely.) The weights $C^{(r)}$ and $D^{(r)}$ are defined similarly. The starting values of these weights are

$$A^{(0)} = \sqrt{x} \ , \tag{102a}$$

$$B^{(0)} = x \ , \tag{102b}$$

$$C^{(0)} = D^{(0)} = 0 \ . \tag{102c}$$

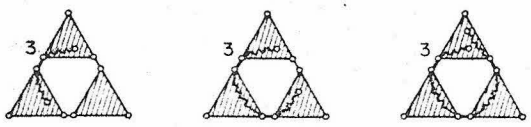


FIG. 11. All possible configurations of an open self avoiding walk of order r. The shaded triangles denote $(r-1)$th order graphs of which only the corner vertices are shown. The factor 3 is for the three possible orientations of the figures.

We call a closed or open walk L of order r if r is the minimum value of p such that the walk can be completely described inside a p^{th} order triangle . The sum of weights of all r^{th} order closed loops inside one r^{th} order triangle is clearly $(B^{(r-1)})^3$. Since there are 3^r points inside each r^{th} order triangle , the contribution of r^{th} order closed loops per site is $3^{-r}(B^{(r-1)})^3$. Hence we get

$$P(x) = \sum_{r=1}^{\infty} 3^{-r} (B^{(r-1)})^3 \quad . \tag{103}$$

Similarly we get (Figure 11)

$$C(x) = \sum_{r=1}^{\infty} 3^{-r} \left[3A^{(r-1)^2} + 3B^{(r-1)} (A^{(r-1)})^2 + 3(B^{(r-1)})^2 D^{(r-1)} \right]. \tag{104}$$

It is easy to write down the recursion equations for the weights $A^{(r)}$, $B^{(r)}$, $C^{(r)}$, $D^{(r)}$ by drawing all possible ways a configuration of an $(r+1)^{th}$ order triangle may arise out of configurations of r^{th} order triangles. Figure 12 shows all possible configurations that contribute to $B^{(r+1)}$. This shows that

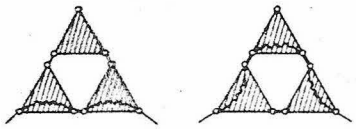


FIG. 12. All possible configurations of rth order triangles (denoted by shaded triangles in the diagram) that contribute to $B^{(r+1)}$.

$$B^{(r+1)} = (B^{(r)})^2 + (B^{(r)})^3 . \qquad (105a)$$

The recursion equations for $A^{(r+1)}$, $C^{(r+1)}$ and $D^{(r+1)}$ are written down similarly (See Appendix C for details) and we get

$$A^{(r+1)} = A^{(r)}(1+2B+2B^2)+C(2B^2) , \qquad (105b)$$

$$C^{(r+1)} = A(B^2) + C(3B^2) , \qquad (105c)$$

$$D^{(r+1)} = (A^2+2A^2B+4ABC+6BC^2) + D(2B+3B^2) . \qquad (105d)$$

We have suppressed the superscripts of $A^{(n)}$, $B^{(n)}$, $C^{(r)}$, $D^{(r)}$ in the right hand sides of Eq.(105b-d).

Equations (102-105) determine the functions C(x) and P(x) completely. We notice that the recursion equation for $B^{(r+1)}$ involves only $B^{(r)}$. Also the recursion equations for $A^{(r+1)}$ and $C^{(r+1)}$ are independent of $D^{(r)}$.

From Eqs. (105a) and (103), we see that P(x) satisfies the functional equation

$$P(x) = x^3/3 + (1/3)\,P(x^2+x^3) . \qquad (106)$$

This equation has fixed points given by the equation

$$x^* = x^{*2} + x^{*3} , \qquad (107)$$

which gives us the fixed points $x^* = 0, (\pm\sqrt{5}-1)/2, \infty$. The fixed points $x^*=0$ and $x^*=\infty$ are attractive fixed points, while the fixed points $x = (\pm\sqrt{5}-1)/2$ are repulsive. The fixed point at $x = (-\sqrt{5}-1)/2$ produces a small even-odd oscillation effect in the coefficients $\overline{P_n}$. Otherwise its

influence on the asymptotic behavior of $\overline{P}_n$ is small, which is essentially determined by the dominant singularity of P(x) closest to the origin at $x=(\sqrt{5}-1)/2$.

If the starting value $B^{(0)}$ is less than $(\sqrt{5}-1)/2$, from Eq. (105a) we see that with successive iterations the value of $B^{(r)}$ decreases to zero. If $B^{(0)}$ is greater than $(\sqrt{5}-1)/2$; for large r , $B^{(r)}$ tends to infinity and P(x) is infinite. This shows that the connectivity constant μ is given by

$$\mu = 2/(\sqrt{5}-1) \approx 1.6180 . \tag{108}$$

Putting $x=1/\mu$ in Eq.(106) we get

$$P(\mu^{-1}) = \mu^{-3}/2 . \tag{109}$$

Consider $x=\mu^{-1}-\delta^{(0)}$, where $\delta^{(0)}$ is a small positive number. Then Eq. (106) gives

$$P(\mu^{-1}-\delta^{(0)}) = \mu^{-3}/3 - \mu^{-2}\delta^{(0)} + (1/3)P(\mu^{-1}-\delta^{(0)}(2+\mu^{-2})) + o(\delta^{(0)2}) . \tag{110}$$

We assume that the singular part of $P(\mu^{-1}-\delta^{(0)})$ varies as $(\delta^{(0)})^{2-\alpha}$. This gives us from Eq. (110)

$$\alpha = 2 - \ell n 3 / [\ell n(2+\mu^{-2})] \approx 0.7342 . \tag{111}$$

Let us define $\delta^{(r)}=\mu^{-1}-B^{(r)}$.

Then to lowest order in $\delta^{(r)}$, Eq. (105a) gives the recursion relation

$$\delta^{(r+1)} = (2+\mu^{-2})\delta^{(r)} . \tag{112}$$

We choose a small positive number ε, and choose a starting value $\delta^{(0)}$ sufficiently small so that

$$1 >> \varepsilon >> \delta^{(0)}, \tag{114}$$

and

$$r_0 \stackrel{def}{=} \ln(\varepsilon/\delta^{(0)})/\ln(2+\mu^{-2}) >> 1 . \tag{115}$$

Then for $r < r_0$, $\delta^{(r)}$ is less than ε and we may replace $B^{(r)}$ in Eqs. (105b- d) by μ^{-1}. This gives us a set of coupled linear recursion equations for the constants A and C

$$A^{(r+1)} \approx A^{(r)}(1+2\mu^{-1}+2\mu^{-2})+C^{(r)}\,2\mu^{-2} , \tag{116a}$$

$$C^{(r+1)} \approx A^{(r)}\,\mu^{-2} \quad +C^{(r)}\,3\mu^{-2} , \tag{116b}$$

which implies that

$$A^{(r)} \propto K_1 \lambda_+^r , \tag{117a}$$

$$C^{(r)} \propto K_2 \lambda_+^r, \qquad \text{for } 1<r<r_0, \tag{117b}$$

where K_1 and K_2 are some constants of proportionality. λ_+ is the larger eigenvalue of the matrix

$$\begin{bmatrix} 1+2\mu^{-1}+2\mu^{-2} & 2\mu^{-2} \\ \mu^{-2} & 3\mu^{-2} \end{bmatrix}, \tag{118}$$

which gives

$$\lambda_+ = [3+3\mu^{-2}+(9-18\mu^{-2}+17\mu^{-4})^{1/2}\,]/2 . \tag{119}$$

Substituting from Eqs. (117a-b) into Eq.(105d), we see that the recursion equation for $D^{(r)}$ has the form

$$D^{(r+1)} \approx K_1 \lambda_+^{2r} + D^{(r)} (2+\mu^{-2}) \ . \qquad (120)$$

Since λ_+^2 is greater than $(2+\mu^{-2})$, this equation implies that

$$D^{(r)} \approx K \lambda_+^{2r} \quad \text{for } 1<r<r_o \ . \qquad (121)$$

For $r>r_o$, the constants $B^{(r)}$ and $C^{(r)}$ approach zero rapidly and $A^{(r)}$ and $D^{(r)}$ tend to finite asymptotic values approximately given by

$$A^{(r)} \approx K(\varepsilon)\lambda_+^{r_o} \ , \text{ for } r>>r_o \ , \qquad (122a)$$

$$D^{(r)} \approx A^{(r)2} \ , \text{ for } r>>r_o \ . \qquad (122b)$$

Here $K(\varepsilon)$ is again a constant of proportionality which depends on ε , but is independent of $\delta^{(o)}$. We substitute these values from Eqs. (122) and (117) into Eq. (104). Approximating the sum by its largest term , we see that

$$C(x) \approx K \left(\lambda_+^2/3\right)^{r_o} . \qquad (123)$$

Substituting for r_o from Eq.(115) we get

$$C(x) \approx K\left(\varepsilon/\Sigma^{(o)}\right)^{\gamma} \ , \qquad (124)$$

with

$$\gamma = \ln(\lambda_+^2/3)/\ln(2+\mu^{-2}) \approx 1.3752 \ . \qquad (125)$$

In Eq.(124) , the constant of proportionality K must vary as $\varepsilon^{-\gamma}$; so that C(x) is independent of ε, as is obvious from its definition.

The critical exponent ν may be determined similarly. We note that for $r<r_o$, the contribution of r^{th} order open loops to R(x) is approximately $(2^{2r})\ K\ (\lambda_+^2/3)^r$. For $r>r_o$, the coefficients $B^{(r)}$ rapidly become zero. In configurations of the type $A^{(r)}$ (Fig. 10) , the end point of the line stays close to the vertex from which it entered the triangle. Thus for $r>r_o$, the contribution of the r^{th} order open loops to R(x) varies as $K(4\lambda_+^2)^{r_o}\ 3^{-r}$. We thus have

$$R(x) \sim K[(4\lambda_+^2)/3]^{r_o} \quad . \tag{126}$$

Substituting for r_o from Eq.(115) and comparing its dependence on $\delta^{(o)}$ with Eq.(100) we get

$$\nu = \ln 2/\ln(2+\mu^2) \approx 0.7986 \quad . \tag{127}$$

This determines all the critical exponents α, γ and ν . We remark here that though a more complete and rigorous analysis of the recursion equations is certainly possible , it is unnecessary since all the constants μ, α, γ , and ν are determined exactly.

Similar analysis may be used to determine the critical exponents for the truncated 4-simplex and the $(2,1)_r$ modified rectangular lattice. The reader is referred to Dhar [45] for details. For the (2,1) modified rectangular lattice , we find that

$$\mu = 1.6909 \ , \ \alpha = 0.6699 \ , \ \gamma = 1.4403 \ , \ \nu = 0.6650 \ . \qquad (128a)$$

And for the truncated 4-simplex lattice

$$\mu = 2.2866 \ , \ \alpha = 0.5413 \ , \ \gamma = 1.4461 \ , \ \nu = 0.7294 \ . \qquad (128b)$$

We note that in all these cases considered here, the critical exponents satisfy the relation

$$d\nu = 2 - \alpha \ , \qquad (129)$$

where d is the dimensionality of the lattice as defined by Nelson and Fisher. On the other hand, we know that in other cases (e.g. the XY model discussed in Sec VII) the dimensionality of the lattice is more usefully defined by the power law behavior of the spectral cumulative distribution function for low frequencies. Perhaps the self-avoiding walks are atypical in that the generating functions whose singularities determine the critical exponents, are not given in terms of the partition function of a Hamiltonian.

The critical behavior of self-avoiding random walks depends strongly on the connectivity properties of the lattice; and not on dimensionality alone. For example, we expect the critical indices α, γ and ν to be different for self avoiding walks on planar and nonplanar two dimensional lattices. This is because planarity determines if the walk can cross itself or not. On the other hand, the critical exponents for the Ising model in two dimensions are

expected to remain unchanged if a small next nearest neighbor interaction is added to the original nearest neighbor Hamiltonian (which makes the lattice nonplanar) .

It is possible to construct pseudo-lattices that have the same effective dimensionality, but different critical exponents for the self avoiding walk problem. Consider , for example, the $(p,1)_p$ modified rectangular lattice. The lattice is planar and has coordination number 3. It may be shown that the effective dimensionality of this lattice is 3/2, independent of p. Also, the dimensionality of the lattice is 2 (again independent of p) if we use Nelson and Fisher's definition. Though the coordination number and the dimensionality of the lattice are independent of p (whichever definition of dimensionality is used), it is easy to verify that the critical exponents for the self avoiding walk problem on these lattices do depend on p. In particular, for p=3 we find that

$$\alpha = 0.6589, \quad \gamma = 1.4601, \quad \nu = 0.6705,$$

which differ from the exponents for p=2 [Eq.(128a)].

It appears that the connectivity structure of these lattices is quite complicated , and a single value of "effective dimensionality" is not sufficient to completely characterize the critical behavior of self avoiding walk problem on these lattices. More study in this area is

needed to identify the parameters that can be used to completely characterize the critical behavior of different Hamiltonians on such pseudo-lattices.

X : CONCLUDING REMARKS

In the preceding discussion we have introduced and studied a class of lattices with effectively nonintegral dimensionality . Although admittedly somewhat artificial , these are of interest in the theory of phase transitions and critical phenomena . They provide a physical basis and testing grounds for techniques such as the ε-expansion , which have up till now remained largely formal. The study of critical behavior of model Hamiltonians on such lattices may be expected to improve our understanding of the influence of dimensionality in determining the nature of phase transitions in physical systems.

These lattices differ in an important way from the axiomatic spaces of nonintegral dimensions defined by Wilson and Stillinger. They are not homogenous , and different lattice points do not have identical neighbourhoods . Homogeneity appears only in a much weaker sense : for any finite neighbourhood of a point , there are infinitely many other points having identical neighbourhoods . This is an important property necessary for the existence of a thermodynamic limit . Also , the magnitude of interaction between different parts of a lattice becomes negligible compared to the magnitude of interaction within parts, as

the volume of parts tends to infinity . The effect of boundary can thus be ignored for sufficiently large systems and the existence of the thermodynamic limit is assured for most physically interesting Hamiltonians on these lattices.

The dimensionality of a lattice cannot be varied continuously in our formulation . To get the critical exponents for a very slightly different value of dimensionality , we have to work with an entirely new lattice, with a new set of recursion equations etc. which have to be analysed afresh . Also it is not possible to construct a lattice with an arbitrary preassigned value d of dimensionality . A little thought shows that this is necessarily so . The lattices which can be contructed using the recursion proccdure described in Section IV , or extentions thereof , are denumerable as their recursive construction has to be describable in a finite number of words. On the other hand , the number of real values of d between any two limits (say, 1 and 2) is nondenumerable . We do , however , have a slightly weaker result (sufficient for most practical purposes) : Dimensionalities of lattices that are described in Section IV , or are formed by forming direct products thereof , form a dense set in the interval $1<d<\infty$.

For lattices with d< 2 , the critical behavior of Hamiltonians can be determined fairly completely using the exact recursion equations. This was illustrated in Sections VII to IX , where the critical behavior of different systems for d<2 lattices was studied . For the classical XY model the critical exponent $\bar{\gamma}$ was shown to be equal to 2/(2-d) . We consider the fact that such simple expressions exist for the critical exponents in terms of the dimensionality of the system , a strong evidence in favor of our definition of dimensionality .

Lattices with d>2 are more interesting because they show nontrivial phase transitions with physically interesting Hamiltonians like the Ising model etc. . In this case, however, the recursion equations usually involve an infinite number of parameters and their exact analysis, and the determination of thermodynamic functions is quite difficult . We may use approximate renormalization equations or numerical extrapolation methods like the series expansions to determine the values of critical exponents . These techniques may also be applied to the study of quantum mechanical Hamiltonians on lattices with d<2 . This seems to be a promising field for furtner investigation .

We studied the critical behavior of self avoiding walks on these lattices, and showed that for lattices with the same value of effective dimensionality , the critical exponents

α, γ, and ν may be different depending on the detailed connectivity properties of the lattice . This shows that the critical exponents are not functions of the dimensionality alone, and series expansions for critical exponents like the ε-expansion should involve additional variables . Even if we adopt the position that the ε-expansion represents the dependence of the critical exponents on dimensionality , "with all other variables held fixed " , it is important to identify these variables explicitly . Lattices with nonintegral effective dimensionality , as defined here , have rather unusual connectivity properties, but if the ε-expansion technique is to be physically meaningful, it should be able to predict the critical exponents for such lattices .

It is hoped that further study of these questions will lead to a better understanding of the influence of dimensionality on phase transitions in general .

PART II

A MODEL OF THE MELTING TRANSITION

I : INTRODUCTION AND OUTLINE

The theory of melting is a longstanding problem of great interest and importance for understanding the physics of solids and liquids. The problem was discussed by Lindemann [46] in an important paper in 1910. He noted that for most materials, the ratio of the root mean square deviation of an atom of a solid just below the melting point and the lattice spacing is approximately constant. Since then, many attempts have been made to present a reasonable theory of the melting transition [47]. The earliest approaches involved evaluating the Gibbs free energy per particle for the fluid and the solid phases separately, and equating them to determine the melting temperature. This approach is still popular and may give results in close agreement with experiments. See, for example, the calculations by Warren and Evenson [48]. This approach is unsatisfactory because it does not treat the fluid and the solid phases on equal footing. Also, it does not help very much in understanding the physics of melting.

Braunbek [49] considered the melting of binary crystals, and supposed that the two sublattices move rigidly with respect to each other. He assumed the mutual potential energy of the lattices to be a periodic function of the displacement. The assumption of perfectly rigid sublattices

is very questionable. Furthermore, it is quite easy to show rigorously that such a model does not undergo any phase transitions.

Lennard-Jones and Devonshire [50] proposed a cell model of melting in which the atoms are localized into cells and move independently of each other in the average field of their neighbors. The theory has since been improved to the "expandable cell" and the "correlated cell" models. For a recent paper employing this approach, see Mori et. al. [51]. This paper treats the correlation between cells in an approximate way. The influence of the approximation on the exact nature of the phase transition is not very clear.

Kirkwood and Monroe [52] found a solid-like solution to the self consistent field equations for the pair distribution function for high densities. The nature of the approximation is , however, not very clear. The approximation is known to be unsatisfactory even for fluids of moderate densities. A somewhat similar, but more reliable, approach to the melting problem is discussed by Ramakrishnan and Youssouff [53].

In the dislocation theories of melting, the solid is assumed to melt when it becomes unstable with respect to spontaneous generation of dislocations [54-55]. This instability criterion has been discussed recently by

Kosterlitz and Thouless [56], Edwards [57], and Nelson [58]. The major objection that may be raised against this approach is that it is a one phase theory. The model does not describe the liquid state.

Much insight into the problem of melting has been gained from the study of computer experiments. The molecular dynamic calculations of Adler and Wainwright [59] showed the existence of a melting transition in hard sphere assemblies as the density of packing is increased. The existence of a phase transition in hard 'sphere' assemblies in lattice and continuum systems has now been proved rigorously using a variant of the Peirls' argument proving the existence of nonzero spontaneous magnetization in Ising magnets at low temperatures [60-61]. Adler and Wainwright observed that the onset of melting in hard sphere assemblies is characterized by the ability of layers to slip past each other.

In the second half of this thesis, we propose a model of the melting transition motivated by the above observation. We consider the thermal motion of a layer of atoms placed in an external periodic potential. The external potential mimics the interaction of the layer with adjacent layers assumed held fixed in their equilibrium configuration. We assume further that interaction between atoms within the layer may be satisfactorily treated in the

harmonic approximation. It is shown that the model undergoes a sharp (albeit continuous) transition from a phase in which the root mean square deviation of atoms in the layer is finite to a phase in which it is infinite, as the temperature of the system is increased. It seems natural to identify these phases as the "solid-like" and the "liquid-like" phases respectively, since the most obvious distinction between solids and liquids is that while in solids the atoms are localized, in liquids they are not. We determine the nature of the transition near the critical point using the renormalization group techniques. Due to the special mathematical structure of the model, we can determine the critical behavior of the model exactly, even though explicit formulas for the free energy, or the exact location of the critical point etc. cannot be determined.

The organization of this second half of our thesis is as follows :

In Section II, we describe the model of melting, and write down a Hamiltonian for it. The Hamiltonian is a lattice version of the Sine-Gordon field theory in two dimensions. We then establish an exact equivalence between the partition function of the melting model , and the grand partition function of a charged lattice gas with a pairwise additive Coulomb-like interaction. The activities of the charges are related to the Fourier coefficients of the

exponential of the periodic potential. We briefly remark on the relationship of this model to the classical XY model in two dimensions, the Kosterlitz-Thouless dislocation melting model, the Kondo problem, and other models related to the above. (For example, the two dimensional superfluid model is related to the classical XY model.)

In Section III, the exact equivalence between the melting model and the charged lattice gas is extended to the case when the melting model is treated quantum mechanically. In this case the behavior of a d-dimensional melting model is related to the behavior of a (d+1) dimensional charged gas where the (d+1)th dimension of the charged gas is continuous and cyclic. The ground state of the d-dimensional quantum-mechanical melting model is related to the finite temperature equilibrium state of a truly (d+1) dimensional classical Coulomb gas, because in this limit, the diameter of the (d+1)th cyclic dimension of the charged gas becomes infinite.

In Section IV, we develop the formalism of the renormalization transformation, applied to the lattice Coulomb gas problem. The degrees of freedom of the system are decreased by a factor of 4 on each renormalization. We use the cumulant expansion techniques to determine the effective Hamiltonian of the system.

The critical behavior of the charged lattice gas is determined in Section V by the analysis of the sequence of effective Hamiltonians obtained by iterating the renormalization transformation. We find that the lattice Coulomb gas undergoes a phase transition at a finite temperature from bound to unbound charges. At low temperatures of the charged gas, the dielectric constant of the gas is finite. Above the critical temperature, it is infinite. It is shown that the specific heat shows a very weak essential singularity, and the correlation length diverges very strongly [$\sim \exp(|T_c - T|^{-1/2})$] near the critical temperature.

Translating these results to the melting problem, we find that the mean square deviation of atoms in the "solid-like" phase varies as $(T_c - T)^{-1/2}$ just below the critical temperature. Above the transition temperature, it is strictly infinite. The specific heat near the transition shows a very weak essential singularity, and the correlation length diverges as $\exp(|T_c - T|^{-\frac{1}{2}})$. We determine the critical temperature for weak perturbing potentials.

In Section VI, the predictions of the model are compared with experiments. We point out the reasons for the shortcomings of the model and suggest some improvements.

II : THE MELTING MODEL AND ITS RELATIONSHIP TO OTHER MODELS IN STATISTICAL MECHANICS

We now describe the model quantitatively. Consider a two dimensional array of atoms, each of mass m_o, forming a square lattice of lattice constant a. The atoms are labelled by a two dimensional integral valued vector $\vec{R} = (m,n)$, where m and n are integers taking values between 1 and M, and 1 and N respectively. The total number of atoms is MN.

With each atom we associate a scalar variable x_{mn} and its canonically conjugate momentum variable p_{mn}. This assumption of scalar variables is made only to simplify notation. The case where the diplacements are vectors may be treated exactly similarly. Later in the section we shall indicate the modifications in the formalism needed to treat the case of vector displacements. The physical properties of the model do not depend on the scalar or vector nature of the displacements. We assume that the interaction between atoms is adequately described within the harmonic approximation. For sake of definiteness, we shall assume that the interaction energy between the atoms of the layer is given by

$$(K/2) \sum_{m,n} [(x_{mn} - x_{m\,m+1})^2 + (x_{mn} - x_{m+1\,n})^2].$$

This assumption is not necessary, and the results are easily

extended to arbitrary harmonic binding between atoms. The Hamiltonian of the system is given by

$$H_o = \sum_{m=1}^{M} \sum_{n=1}^{N} [\, p_{mn}^2 /(2m_o) + (K/2)\{(x_{mn} - x_{m\,n+1})^2 + (x_{mn} - x_{m+1\,n})^2\}] \tag{1}$$

This is a standard problem in classical mechanics. The Hamiltonian can be diagonalized by a change of variables to coordinates $p_{\bar{k}}$ and $q_{\bar{k}}$, where $p_{\bar{k}}$ and $q_{\bar{k}}$ are Fourier transforms of the coordinates p_{mn} and x_{mn}. We get

$$H_o = \sum_{\bar{k}} [\, p_{\bar{k}}^* p_{\bar{k}} /(2m_o) + K(2 - \cos k_x - \cos k_y) q_{\bar{k}}^* q_{\bar{k}} \,], \tag{2}$$

where $\vec{k} = (k_x, k_y)$, and k_x and k_y take the values $2\pi r/M$ and $2\pi s/N$ respectively. ($r = -M/2$ to $M/2 - 1$; $s = -N/2$ to $N/2 - 1$). The partition function for this problem is easily written down. We get

$$Z_o = \prod_{m,n} \left(\int_{-\infty}^{+\infty} dp_{mn} \int_{-\infty}^{+\infty} dx_{mn} \right) \exp[-\beta H_o] \tag{3}$$

$$= \prod_{\bar{k}} (2\pi / \beta \omega_{\bar{k}}), \tag{4}$$

where $\omega_{\bar{k}}$ is the frequency of the mode labelled by the wave vector $\bar{k}$. It is easy to see that

$$\omega_{\bar{k}}^2 = (2K/m_o)\,(2 - \cos k_x - \cos k_y) \,. \tag{5}$$

We now perturb the system by placing it in an external periodic potential having the same periodicity as the lattice. Physically, the periodic potential imitates the interaction of this layer with adjacent layers in a three dimensional solid. We hold the adjacent layers fixed, and study the motion of only one layer. The interaction energy

of each atom (m,n) due to the perturbing potential is a periodic function of x_{mn}. We choose the periodic function to be a cosine function for simplicity. Then, the full Hamiltonian of this layer of harmonically bound atoms placed in an external periodic potential is given by

$$H = H_o + H_1 , \tag{6}$$

where

$$H_1 = -V_o \sum_{m,n} \cos(2\pi x_{mn}/a). \tag{7}$$

The partition function for the perturbed problem is given by

$$Z = Z_o \langle \exp(-\beta H_1) \rangle_{H_o} , \tag{8}$$

where the angular brackets denote thermodynamic averaging with respect to the unperturbed Hamiltonian H_o. We recall the identity

$$\exp(x \cos\theta) = \sum_{q=-\infty}^{+\infty} I_q(x) \exp(i q \theta), \tag{9}$$

where $I_q(x)$ is the modified Bessel's function of argument x and of order q. Making use of this identity we may write

$$\exp(-\beta H_1) = \sum_{\{q_{mn}\}} \{ \prod_{m,n} I_{q_{mn}}(\beta V_o) \} \exp[2\pi i \sum_{mn} q_{mn} x_{mn}/a]. \tag{10}$$

Now, under H_o the variables $\{x_{mn}\}$ are distributed normally. A linear combination of these variables $2\pi \sum_{mn} x_{mn} q_{mn}$ is also a Gaussian random variable. We recall that for a Gaussian random variable ξ

$$\langle \exp(i\xi) \rangle = \exp(-\langle \xi^2 \rangle/2). \tag{11}$$

Using this result to evaluate the expectation value in Eq.(8) we get

$$Z/Z_0 = \sum_{\{q_{mn}\}} \exp(-\tilde{\beta}\tilde{H}), \tag{12}$$

where we have put

$$\tilde{H} = -(1/\tilde{\beta}) \sum_{mn} \ln I_{q_{mn}}(\beta V_0) - (1/2) \sum_{(m,n)\neq(m',n')} q_{mn} q_{m'n'} \Phi(m,n;m',n'), \tag{13}$$

$$\Phi(m,n;m',n') = \Phi(m-m',n-n')$$

$$= \int_{-\pi}^{+\pi} \frac{dk_x}{2\pi} \int_{-\pi}^{+\pi} \frac{dk_y}{2\pi} \frac{[1-\cos\{(m-m')k_x + (n-n')k_y\}]}{2-\cos k_x - \cos k_y}, \tag{14}$$

and

$$\tilde{\beta} = K_B T \pi^2/(Ka^2). \tag{15}$$

The right hand side of Eq.(12) is seen to be interpretable as the grand partition function of a charged lattice gas. At each site (m,n) we have a discrete charge q_{mn}. The Hamiltonian consists of a pairwise additive interaction between charges, bilinear in the charges, and a chemical potential term.

In Eq.(12), the summation over the configurations of charges $\{q_{mn}\}$ has been restricted to the case when $\sum_{mn} q_{mn} = 0$. It is easy to see that all other configurations have zero weight in the statistical sum. In the charged lattice gas language we say that it takes an infinite amount of energy to create isolated charges, and hence all configurations satisfy the overall charge neutrality

condition $\sum_{mn} q_{mn} = 0$.

From the defining equation (14), it is easy to verify that the potential $\Phi(R)$ is long-range and varies as $(1/\pi)\ell n(R)$ for large separations R. This is in keeping with our interpretation of $\Phi(R)$ as the two dimensional electrostatic potential between the the charges $\{q_{mn}\}$.

Let us now briefly indicate the modifications to the above equivalence needed when we consider more general interactions than discussed above. It is easy to verify that the equivalence holds for arbitrary lattice structure and arbitrary dimensionality of the lattice. We may introduce next nearest neighbor quadratic interaction, or any other quadratic interaction in H_o. The result only changes the functional dependence of ω_k on $\bar{k}$. In each case, the potential Φ is related to the Fourier transform of $(1/\omega_k^2)$. Also, so long as ω_k^2 is proportional to k^2 for small k, the potential $\Phi(R)$ is logarithmic for large separations R in two dimensions.

We may introduce a more general functional form for the periodic potential than the cosine dependence assumed in Eq.(7). This only changes the activities $I_q(\beta V_o)$ of the charged gas. They are no longer Bessel's functions of order q, but somewhat more general functions of q.

Finally, we may consider vector displacements. In this case we have to introduce two species of charges, one for each component of the vector displacement. The charged gas has two species of charges; at each site (m,n) , we have two integer valued charge variables q_{1mn} and q_{2mn}. The electrostatic interaction between the charges may be written down easily, and has the form

$$-(1/2)\sum_{\alpha,\alpha'=1}^{2}\sum_{(m,n)\neq(m'n')} q_{\alpha mn}\, q_{\alpha' m'n'}\, \Phi_{\alpha\alpha'}(m,n;m',n').$$

The interaction potential $\Phi_{\alpha\alpha'}$ is small unless $\alpha=\alpha'$. If we ignore the interspecies interaction of the charges, the problem just becomes a problem of two independent single species charged gases interpenetrating each other. Hence the critical behavior is the same as it would be if the displacements were scalars. This argument can be made more rigorous. It is possible to show that the interspecies interaction $\Phi_{\alpha\alpha'}$ is an "irrelevant" operator under the renormalization transformation discussed in Section IV. The term "irrelevant" means that the interaction may be ignored without affecting the critical behavior.

We have thus established the equivalence of the melting model and the classical lattice Coulomb gas. In two dimensions, the potential of interaction is logarithmic for the charged lattice gas. This interaction is of great interest in statistical physics and many different systems

may be modelled by it.

Kosterlitz and Thouless [56] and Feynman [62] have discussed a dislocation model of two dimensional melting. In two dimensions, the lattice dislocations have interaction energy which increases logarithmically with separation. A similar situation arises in two-dimensional superfluids, where the interaction energy of vortex-pair excitations increases logarithmically with the distance between them. If the variation of the amplitude of the superfluid wave function is considered to be small compared to its variation in phase, the two dimensional superfluidity problem is equivalent to the classical XY model. Finally, it has been shown that four dimensional abelian lattice gauge field theories have similar renormalization properties [63] and similar "instanton" structures as the classical XY model in two dimensions [64].

Anderson and Yuwal have treated the Kondo problem in [65]. In the Kondo problem, we study the behavior of isolated magnetic impurities which may interact with electrons in the conduction band. This problem may be converted to a one dimensional continuum problem of an interacting charged gas where the charges are alternately positive and negative and interact with each other by a long range logarithmic interaction. While this problem is one dimensional, the important property of the interaction

potential being logarithmic at large separations implies that techniques similar to those for the two dimensional charged gas, may be applied here too with minor modifications. The critical behavior of the two systems is very similar. Also, the Kondo problem is equivalent to a one dimensional Ising model with longrange interaction varying as R^{-2} , where R is the distance between spins [66].

Finally, we note that the melting model is clearly a fairly good model of a monolayer adsorbed on a crystalline substrate, having the same periodicity as the substrate.

We thus see that our melting model is related to many important problems in the field of phase transitions and critical phenomena, and deserves much attention.

III : EQUIVALENCE OF THE QUANTUM MECHANICAL MELTING MODEL TO A CLASSICAL COULOMB GAS

In this section we extend the equivalence between the system of coupled simple harmonic oscillators in an external periodic potential and the classical Coulomb gas, to the case where the oscillators are treated quantum mechanically. It is shown that the evaluation of the free energy of a d-dimensional quantum mechanical melting model is equivalent to the evaluation of the Landau potential of a (d+1) dimensional classical Coulomb gas. The space of the charged Coulomb gas is discrete in d dimensions forming a lattice same as the lattice formed by the coupled harmonic oscillators, but the (d+1)th dimension is continuous and cyclic. The pairwise additive interaction between the charges is shown to be Coulomb-like, though it is slightly temperature dependent. In the limit of high temperatures for the melting model, the quantum mechanical effects are unimportant and we reproduce the classical result. In the limit of zero temperature of the melting model, we get a truly (d+1) dimensional charged gas, in the sense that the (d+1)th dimension is also infinite in extent.

We consider a d-dimensional "simple cubic" lattice, and start with the Hamiltonian

$$H = H_0 + H_1 \ , \tag{16}$$

$$H_0 = \sum_{\bar{k}} [p_{\bar{k}}^* \, p_{\bar{k}} \, /(2m_0) + (1/2) m_0 \omega_{\bar{k}}^2 q_{\bar{k}}^* \, q_{\bar{k}}], \tag{17}$$

$$H_1 = -V_0 \sum_{\bar{R}} \cos(2\pi x_{\bar{R}} \, / a \ ) \ . \tag{18}$$

Here $x_{\bar{R}}$ is the displacement from equilibrium of the atom whose equilibrium position is at site $\bar{R}$. (We treat different atoms as distinguishable.) $\bar{R}$ is a d-dimensional integer valued vector. $p_{\bar{k}}$ and $q_{\bar{k}}$ are the momentum and the coordinate of the normal mode labeled by the wave vector $\vec{k}$. The total number of sites in the lattice is N. a is the lattice constant and for simplicity, we have considered scalar displacements. Generalization to vector displacements is immediate.

The coordinates $x_{\bar{R}}$ and $q_{\bar{k}}$ are of course related by

$$q_{\bar{k}} = (1/\sqrt{N}) \sum_{\bar{R}} x_{\bar{R}} \ \exp(-i\vec{k}\cdot\vec{R}) \ , \tag{19}$$

$$x_{\bar{R}} = (1/\sqrt{N}) \sum_{\bar{k}} q_{\bar{k}} \ \exp(i\vec{k}\cdot\vec{R}). \tag{20}$$

Putting

$$q_{\bar{k}} = (\hbar/2m_0\omega_{\bar{k}})^{1/2} \ (\ a_{-\bar{k}} + a_{\bar{k}}^+ \ ), \tag{21}$$

and

$$p_{\bar{k}} = -i \, (\hbar m_0 \omega_{\bar{k}} /2)^{1/2} \ (\ a_{-\bar{k}} - a_{\bar{k}}^+ \ ), \tag{22}$$

we get

$$H_0 = \sum_{\vec{k}} \hbar\omega_{\vec{k}} (a^+_{\vec{k}} a_{\vec{k}} + 1/2) , \tag{23}$$

and

$$[a_k , a^+_{k'}] = \delta_{k,k'} . \tag{24}$$

We work in the interaction picture and define

$$S(\beta) = \exp(\beta H_0) \exp(-\beta H)$$

$$= T \exp[-\int_0^\beta d\beta' H_1(\beta')], \tag{25}$$

where

$$H_1(\beta') = \exp(\beta' H_0) H_1 \exp(-\beta' H_0), \tag{26}$$

and T is the β-ordering operator. Then we get

$$Z = Tr \exp(-\beta H) = Tr[\exp(-\beta H_0) S(\beta)], \tag{27}$$

and

$$Z' \overset{def}{=} Z / Z_0$$

$$= [Z_0]^{-1} \cdot Tr \exp(-\beta H_0) \cdot \left[\sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^\beta d\beta_1 \int_0^\beta d\beta_2 \cdots \int_0^\beta d\beta_n \, T H_1(\beta_1) H_1(\beta_2) \cdots H_1(\beta_n)\right] \tag{28}$$

We have defined Z_0 to be the unperturbed partition function corresponding to the Hamiltonian H_0. We further define

$$\xi_{\vec{R}}(\beta') = \exp(\beta' H_0) (2\pi x_{\vec{R}} / a) \exp(-\beta' H_0) ,$$

$$= \sum_{\vec{k}} \frac{2\pi}{a} \sqrt{\frac{\hbar}{2 m_0 \omega_{\vec{k}} N}} \left(a_{\vec{k}} e^{-i\vec{k}\cdot\vec{R} - \beta'\omega_{\vec{k}}} + a^+_{\vec{k}} e^{+i\vec{k}\cdot\vec{R} + \beta'\omega_{\vec{k}}} \right) \tag{29}$$

Substituting $\cos(2\pi x_{\vec{R}}/a) = \frac{1}{2}\sum_{\eta=\pm 1} \exp(2\pi x_{\vec{R}} i\eta/a)$, into Eq.(28) we get

$$Z' = Z_0^{-1} \sum_{n=0}^{\infty} \left(\frac{V_0}{2}\right)^n \frac{1}{n!} \left[\prod_{i=1}^{n} \left\{ \sum_{R_i} \int_0^\beta d\beta_i \sum_{\eta_i=\pm 1} \right\} \right.$$

$$\left. \cdot Tr \, T \left\{ \exp(-\beta H_0) \exp(i\eta_1 \xi_1) \exp(i\eta_2 \xi_2) \cdots \exp(i\eta_n \xi_n) \right\} \right]. \tag{30}$$

where we have abbreviated $\xi_{\vec{R}_i}(\beta_i) = \xi_i$. Using the operator identities

$$(\exp A)(\exp B) = \exp(A+B)\exp[A,B/2] , \tag{31}$$

and

$$\mathrm{Tr}\exp(-\lambda a^\dagger a)\exp(\mu a^\dagger)\exp(\nu a) = \{1-e^{-\lambda}\}^{-1}\exp\left(\frac{\mu\nu}{e^\lambda-1}\right), \tag{32}$$

it is easy to evaluate the trace in Eq.(30), and one gets

$$Z' = \sum_{n=0}^{\infty}\left(\frac{\nu_0}{2}\right)^n\frac{1}{n!}\left[\left\{\prod_{i=1}^{n}\left(\sum_{\vec{R}_i}\int_0^\beta d\beta_i\sum_{\eta_i=\pm1}\right)\right\}\exp\left\{-\frac{1}{2}\sum_{i,j=1}^{n}\eta_i\eta_j\,\Phi(\vec{R}_i,\beta_i;\vec{R}_j,\beta_j)\right\}\right] \tag{33}$$

where

$$\Phi(\vec{R}_i,\beta_i;\vec{R}_j,\beta_j) = \frac{1}{N}\sum_{\vec{k}}\frac{2\pi^2}{a^2}\frac{\hbar}{m\omega_k}\cosh\left(\frac{\beta}{2}-|\beta_i-\beta_j|\right)\hbar\omega_k\cdot\mathrm{cosech}\,\frac{\beta\hbar\omega_k}{2}\cdot\exp[i\vec{k}\cdot(\vec{R}_i-\vec{R}_j)] \tag{34}$$

$$= \langle T\,\xi_i\xi_j\rangle_{H_0} \tag{35}$$

as may be easily verified.

Thus Z' is seen to be the grand partition function of a classical charged gas with pairwise additive interactions. The position of the ith charge is specified by the (d+1) coordinates $(\vec{R}_i,\beta_i)$, where the last coordinate is continuous $0\le\beta_i\le\beta$. The pair potential is invariant under translation and reflections and has the additional property that

$$\Phi(\vec{R}_i,\beta_i;\vec{R}_j,\beta_j) = \Phi(\vec{R}_i,\beta-\beta_i+2\beta_j;\vec{R}_j,\beta_j). \tag{36}$$

This shows that we can treat the coordinate β_i as a cyclic coordinate. The summations over $\vec{R}_i$ and the integrations over β_i in Eq.(33) are thus to be understood as integrations over all positions of a charge in the (d+1) dimensional space.

To understand the pair potential better, we look at its Fourier transform. Since the β coordinate is cyclic, the corresponding Fourier transform variable is discrete. We get

$$\Phi(\vec{R}_i - \vec{R}_j, \beta_i - \beta_j) = (2\pi^2 k_B T/m_e a^2 N) \sum_{\vec{k},\theta} \frac{e^{i\vec{k}\cdot(\vec{R}_i - \vec{R}_j) + i\theta(\beta_i - \beta_j)}}{\omega_{\vec{k}}^2 + \theta^2} \quad . \tag{37}$$

Here the summations over $\vec{k}$ are essentially continuous, (equivalent to integrations over the first Brillouin zone). but the summation over θ is a summation over a discrete set of values $\theta = 2\pi r/(\hbar\beta)$, r integral, which remains discrete even if the size of the lattice tends to infinity.

We see that the Fourier transform of the potential is of the form $(1/q^2)$, where q^2 is the (d+1) dimensional momentum transfer.

Since the spacing between the allowed values of θ is proportional to the temperature, we see that the interaction is temperature dependent. Of special interest are the limits $\beta \longrightarrow 0$ and $\beta \rightarrow \infty$. In the high temperature limit of the melting model, the radius of the cylindrical dimension for the charged gas shrinks to zero. The interaction energy between the charges in this limit becomes independent of their β coordinate. Integrations over the coordinates β_i may then be done trivially, to give a multiplicative factor β for each charge, and we recover the classical case discussed in the previous section.

In the case $\beta \to \infty$, the summation over θ in Eq.(37) tends to a continuous integral and we get a (d+1) dimensional Coulomb gas. This is particularly interesting because we observe that the quantum mechanical melting model in one dimension is equivalent to a Coulomb-like classical gas in two dimensions. As we shall show, the two dimensional Coulomb gas undergoes a phase transition. After an appropriate identification of symbols, we find that a "mobile-immobile" transition occurs in one dimensional chains in a weak external periodic potential at a critical value of the mass per atom $m_c \simeq \hbar\pi/(4ac)$. Here c is the velocity of sound in the chain and a is the lattice spacing. If the mass per atom $m_o < m_c$, in the ground state of the one dimensional system, each particle has an infinite root mean square deviation. For masses $m_o > m_c$, the particles become bound by the periodic potential and the root mean square deviation of the particles is finite.

The behavior of other quantities of interest (e.g. correlation length, elementary excitations etc.) may be deduced from the behavior of corresponding quantities for the two dimensional Coulomb gas at finite temperature. We shall determine these using the renormalization group techniques in the next two sections.

IV : RENORMALIZATION GROUP TREATMENT OF THE LATTICE COULOMB GAS PROBLEM

In this section we shall determine the critical behavior of the two dimensional lattice Coulomb gas problem using renormalization group techniques. The treatment in this section and the next one is fairly self contained and for the most part can be read independently of the rest of this thesis.

The two dimensional continuum Coulomb gas has been studied by Hauge and Hemmar [67], Salzburg and Prager [68], and May [69]. For the continuum case we can determine the exact equation of state using scaling arguments, even though the partition function cannot be evaluated as a function of temperature. The continuum model is somewhat unphysical, because the classical partition function diverges below the critical temperature. Hauge and Hemmar considered the problem of a two dimensional gas of charged disks with hardcore radius a. In the limit of the hardcore radius going to zero, they obtained the equation of state

$$P = nk_B (T - T_c/2) \qquad \text{for } T \geq T_c , \tag{38a}$$

$$= nk_B T/2 \qquad \text{for } T \leq T_c . \tag{38b}$$

Here P is the pressure of the gas and n is the number density of the charged disks.

However, if a is finite, the scaling argument does not work and the problem is difficult to solve. In particular, the nature of the phase transition is difficult to determine.

Kosterlitz [70] has studied the two dimensional Coulomb gas problem with ultraviolet cutoff, in the context of the classical XY model, and showed that the phase transition involves an exponentially diverging correlation length near the critical point, with an essential singularity in specific heat. Earlier, a similar phase transition was found by Anderson and Yuwal [65] in the Kondo problem. In fact, the renormalization equations for these problems are very similar. More recently, Nelson [58] has studied the Kosterlitz-Thouless dislocation transition in two dimensional films. He has shown that on a triangular lattice, the dependence of the correlation length near critical temperature is modified to $\exp(A|T-T_c|^{-2/5})$. (Here A is some constant.) This arises due to the geometric fact that on a triangular lattice, three Burger vectors of unit magnitude may add up to a zero sum. A similar situation does not arise in our model, and we shall show that near the transition temperature, the correlation length varies as $\exp(A|T-T_c|^{-\frac{1}{2}})$.

A somewhat similar result for the two dimensional field theory was obtained by Coleman [71]. He showed that the 1x-1t dimensional scalar field theory with self-interaction density proportional to $\cos(\beta\Phi)$ is equivalent to the charge zero sector of the massive Thirring model. However, since he does not incorporate any ultravoilet cutoff, the theory is ill defined for $\beta > 8\pi$. This result is, of course, equivalent to the divergence of the classical partition function of a two dimensional continuum Coulomb gas for temperatures below the critical temperature.

The Hamiltonian of the two dimensional lattice Coulomb gas is given by

$$H = -(1/2)\sum_{i,j} q_i\, q_j\, \Phi(\vec{i}-\vec{j}) - (1/\beta)\sum_i \ln I(q_i) \,, \qquad (39)$$

where

$$\Phi(\vec{i}-\vec{j}) = \int_{-\pi}^{\pi}\frac{dk_x}{2\pi}\int_{-\pi}^{\pi}\frac{dk_y}{2\pi}\,\frac{[1-e^{i\vec{k}\cdot(\vec{i}-\vec{j})}]}{2-\cos k_x-\cos k_y} \,, \qquad (40)$$

is the pairwise additive two body Coulomb potential. $\vec{i}$ and $\vec{j}$ are two dimensional lattice vectors denoting the position of lattice sites, $\vec{i}=(i_1, i_2)$ and $\vec{j}=(j_1, j_2)$. q_i is an integer valued variable denoting the charge at site $\vec{i}$. The second term in the Hamiltonian represents the chemical potential for the charges $\{q_i\}$. The corresponding chemical activities $I(q_i)$ satisfy the charge inversion symmetry relations

$$I(q) = I(-q) , \tag{41}$$

but are otherwise arbitrary. Without any loss of generality, we assume that $I(0) = 1$. β is the inverse temperature.

The thermodynamic properties of the system are determined by the grand canonical partition function of the system

$$Z = \sum_{\{q_i\}} \exp(-\beta H) , \tag{42}$$

where the summation extends over all configurations $\{q_i\}$ of the charges q_i, subject to the constraint that $\sum_i q_i = 0$. If $\sum_i q_i \neq 0$, we define the energy of the configuration to be infinite, so that the weight of the configuration in the configuration sum becomes zero. This corresponds to the fact that in two dimensions, an infinite amount of energy is required to create isolated charges.

The critical properties of the system are determined using the renormalization procedure. We group the lattice sites into blocks of 2×2 sites each. The lattice sites are now specified by a block coordinate $\alpha = (\alpha_1, \alpha_2)$, where α_1 and α_2 are integers; and an internal index m taking values from 1 to 4 [Fig. 13].

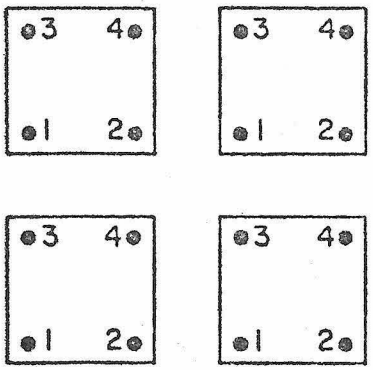


FIG. 13. The renormalization transformation. Each block of 2x2 spins is replaced by a single site. The internal index m (m goes from 1 to 4) is used to specify individual sites within a particular block.

Also, instead of the site variables $q_i \equiv q_{\alpha,m}$, we define new block variables Q_α and $S_{\alpha,p}$ (p=1 to 3) by the equations

$$Q_\alpha = q_{\alpha,1} + q_{\alpha,2} + q_{\alpha,3} + q_{\alpha,4} \quad , \tag{43a}$$

$$S_{\alpha,1} = q_{\alpha,1} + q_{\alpha,2} - q_{\alpha,3} - q_{\alpha,4} \quad , \tag{43b}$$

$$S_{\alpha,2} = q_{\alpha,1} - q_{\alpha,2} + q_{\alpha,3} - q_{\alpha,4} \quad , \tag{43c}$$

$$S_{\alpha,3} = q_{\alpha,1} - q_{\alpha,2} - q_{\alpha,3} + q_{\alpha,4} \quad . \tag{43d}$$

The variables Q_α , $S_{\alpha,1}$, $S_{\alpha,2}$, $S_{\alpha,3}$ measure the total charge, the two components of the dipole moment and the quadrupole moment of the block α respectively. Since $q_{\alpha,m}$ are

integers, we see that Q_α may take arbitrary integral values, but the values of the variables $S_{\alpha,p}$ (p=1 to 3) depend on Q_α. In particular, $S_{\alpha,p}$ are constrained to have the same parity as Q_α. In terms of these block variables, the Hamiltonian of Eq.(39) may be rewritten as

$$H = H_0 + H_1 + H_2, \tag{44}$$

with

$$H_0 = -(1/2)\sum_{\alpha\neq\beta} Q_\alpha Q_\beta \Psi_{QQ}(\alpha,\beta) - (1/\beta)\sum_{\alpha,m} \ln I(q_{\alpha,m}) - (1/2)\sum_{\alpha}\sum_{m_1\neq m_2} q_{\alpha,m_1} q_{\alpha,m_2} \Phi(\alpha,m_1;\alpha,m_2) \tag{45}$$

$$H_1 = \sum_{p=1}^{3}\sum_{\alpha\neq\beta} Q_\alpha S_{\beta,p} \Psi_{Qp}(\alpha,\beta), \tag{46}$$

$$H_2 = \sum_{p,q=1}^{3}\sum_{\alpha\neq\beta} S_{\alpha,p} S_{\beta,q} \Psi_{pq}(\alpha,\beta). \tag{47}$$

Here we have defined

$$\Psi_{QQ}(\alpha,\beta) = (1/16)\sum_{m_1=1}^{4}\sum_{m_2=1}^{4} \Phi(\alpha,m_1;\beta,m_2), \tag{48}$$

and

$$\Psi_{Q1}(\alpha,\beta) = (1/16)\sum_{m=1}^{4}[\Phi(\alpha,m;\beta,1) + \Phi(\alpha,m;\beta,2) - \Phi(\alpha,m;\beta,3) - \Phi(\alpha,m;\beta,4)]. \tag{49}$$

Similar expressions for the potentials Ψ_{Qp} and Ψ_{pq} (p,q=1 to 3) in terms of $\Phi(\vec{i},\vec{j})$ are easily written down. The restriction $\alpha\neq\beta$ in Eqs.(46) and (47) may be removed if we define

$$\Psi_{Qp}(\alpha,\alpha) = \Psi_{pq}(\alpha,\alpha) = 0. \tag{50}$$

The potential $\Phi(\vec{\imath}-\vec{\jmath})$ is long range and behaves logarithmically for large separations $|\vec{\imath}-\vec{\jmath}|$. From the defining equation (40), it is easy to see that for large separations $|\vec{\imath}-\vec{\jmath}|$

$$\Phi(\vec{\imath},\vec{\jmath}) \approx (1/\pi)[\ln|\vec{\imath}-\vec{\jmath}| + \gamma + (3/2)\ln 2] + O(\tfrac{1}{|\vec{\imath}-\vec{\jmath}|}), \quad (51)$$

where γ is Euler's constant. The potentials $\Psi_{Qp}(\alpha,\beta)$, $\Psi_{Q3}(\alpha,\beta)$, $\Psi_{Pq}(\alpha,\beta)$, $\Psi_{P3}(\alpha,\beta)$ and $\Psi_{33}(\alpha,\beta)$ (p,q=1,2) may be similarly shown to vary as R^{-1}, R^{-2}, R^{-2}, R^{-3}, and R^{-4} respectively for large separations $R=|\alpha-\beta|$. For example, $\Psi_{33}(\alpha,\beta)$ is the quadrupole-quadrupole interaction in two dimensional electrostatics, and hence decreases with distance as R^{-4}. Also, these potentials are well behaved and remain finite for small separations. We expect the overall influence of H_1 and H_2 to be small compared to H_0, and hence these interactions may be usefully treated as small perturbations.

We now sum over the variables $\{S_{\alpha,p}\}$ (p=1 to 3) in the expression for the grand partition function [Eq.(42)]. This gives us an expression which is proportional to the marginal probability distribution of the variables $\{Q_\alpha\}$. We may define an effective Hamiltonian for the variables $\{Q_\alpha\}$ by the equation

$$\exp[-\beta_{eff} H_{eff}\{Q_\alpha\}] = \sum_{\{S_{\alpha,p}|Q_\alpha\}} \exp[-\beta H]. \quad (52)$$

Here the summation extends over all possible values of $\{S_{\alpha,p}\}$ consistent with the configuration of block charges $\{Q_\alpha\}$. In this equation β_{eff} is an arbitrary constant fixing the scale of the effective Hamiltonian H_{eff}. We shall make a specific choice of β_{eff} later in the discussion.

We use the cumulant expansion technique to write down an explicit series expansion for $H_{eff}\{Q_\alpha\}$ in powers of H_1 and H_2. This is done by first writing the exponential of $\beta_{eff} H_{eff}\{Q_\alpha\}$ as a power series in the perturbation $(H_1 + H_2)$. Then we take the logarithm of this series to determine a power series for $\beta_{eff} H_{eff}\{Q_\alpha\}$ in powers of $(H_1 + H_2)$.

From Eqs. (44) and (52) we write

$$\exp[-\beta_{eff} H_{eff}] = \sum_{\{S_{\alpha p}|Q_\alpha\}} \exp\left[-\beta H_0(\{Q_\alpha, S_{\alpha p}\})\right] \left[\sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} (H_1+H_2)^n\right]$$

$$= \left[\sum_{\{S_{\alpha p}|Q_\alpha\}} \exp\left[-\beta H_0(\{Q_\alpha, S_{\alpha p}\})\right]\right] \cdot \left[\sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \left\langle (H_1+H_2)^n \right\rangle_{H_0,\{Q_\alpha\}}\right] \quad (53)$$

where we have used the notation

$$\left\langle \mathcal{O} \right\rangle_{H_0,\{Q_\alpha\}} = \left[\sum_{\{S_{\alpha p}|Q_\alpha\}} \exp[-\beta H_0]\, \mathcal{O}\right] \cdot \left[\sum_{\{S_{\alpha p}|Q_\alpha\}} \exp\left[-\beta H_0(\{Q_\alpha, S_{\alpha p}\})\right]\right]^{-1} \quad (54)$$

for any thermodynamical variable $\mathcal{O} = \mathcal{O}(\{Q_\alpha, S_{\alpha p}\})$. The angular brackets represent the thermodynamic average value of the variable in an ensemble with probability distribution corresponding to the Hamiltonian H_0, subject to the constraint that the block charges at sites α are fixed at

values Q_α.

Under H_0, the variables $S_{\alpha,p}$ at different blocks α are independent of each other, and the summations are easily done. We define

$$\bar{I}(Q_\alpha) = \sum_{\{S_{\alpha,p}|Q_\alpha\}} \exp\Big[\sum_m \ln I(q_{\alpha,m}) - (1/2)\sum_{m_1 \neq m_2} q_{\alpha,m_1} q_{\alpha,m_2} \Phi(\alpha,m_1;\alpha,m_2)\Big] \quad (55)$$

Then we get

$$\sum_{\{S_{\alpha,p}|Q_\alpha\}} \exp\Big[-\beta H_0(\{Q_\alpha, S_{\alpha,p}\})\Big] = \exp\Big[-\frac{\beta}{2}\sum_{\alpha\neq\beta} Q_\alpha Q_\beta \Psi_{QQ}(\alpha,\beta) + \sum_\alpha \ln \bar{I}(Q_\alpha)\Big]. \quad (56)$$

The moments of H_1 and H_2 about this distribution are easily taken. We write

$$\langle S_{\alpha,1}^{2m} S_{\alpha,2}^{2n} S_{\alpha,3}^{2p} \rangle_{H_0,\{Q_\alpha\}} = \mu_{2m,2n,2p}(Q_\alpha), \quad (57a)$$

and

$$\langle S_{\alpha,1}^{2m+1} S_{\alpha,2}^{2n+1} S_{\alpha,3}^{2p+1} \rangle_{H_0,\{Q_\alpha\}} = \mu_{2m+1,2n+1,2p+1}(Q_\alpha). \quad (57b)$$

Here m,n and p are integers. All other powers of $S_{\alpha,p}$ on the same block α have zero expectation value by symmetry. Since $S_{\alpha,p}$ at different blocks are uncorrelated, all the expectation values in Eq. (53) may be written down in terms of the moments $\mu_{m,n,p}(Q_\alpha)$. For example, we have

$$\langle H_1 + H_2 \rangle = 0, \quad (58)$$

$$\langle (H_1+H_2)^2 \rangle = \sum_{\alpha,\beta,\gamma}\sum_{p=1}^{3} Q_\alpha Q_\beta \mu_{2\delta_{p1},2\delta_{p2},2\delta_{p3}}(Q_\gamma)\Psi_{Qp}(\alpha,\gamma)\Psi_{Qp}(\beta,\gamma)$$
$$+2\sum_{\alpha,\beta}\sum_{p,q=1}^{3} \mu_{2\delta_{p1},2\delta_{p2},2\delta_{p3}}(Q_\alpha)\mu_{2\delta_{q1},2\delta_{q2},2\delta_{q3}}(Q_\beta)[\Psi_{pq}(\alpha,\beta)]^2. \quad (59)$$

Here δ is the Kronecker delta symbol. Expressions for higher order moments may be written down similarly. All the moments are functions of $\{Q_\alpha\}$ only, since all the dependence on $\{S_{\alpha,p}\}$ has been integrated out. The

expressions for these moments are substituted in Eq.(53). We take the logarithm of this series and write it as as an exponential of an infinite series in powers of H_1 and H_2 using the cumulant expansion. We note that $\langle (H_1 + H_2) \rangle_{H_0,\{Q_\alpha\}}$ is zero, and the cumulant expansion may be written as

$$\sum_{n=0}^{\infty} (-\beta)^n \langle (H_1 + H_2)^n \rangle_{H_0,\{Q_\alpha\}} / n!$$
$$= \exp[(\beta^2/2) \langle (H_1 + H_2)^2 \rangle_{H_0,\{Q_\alpha\}} + (\beta^3/6) \langle (H_1 + H_2)^3 \rangle_{H_0,\{Q_\alpha\}}$$
$$+ (\beta^4/24) \{ \langle (H_1 + H_2)^4 \rangle_{H_0,\{Q_\alpha\}} - 3 \langle (H_1 + H_2)^2 \rangle^2_{H_0,\{Q_\alpha\}} \}$$
$$+ \text{higher order cumulants}] . \qquad (60)$$

All these cumulants are functions of $\{Q_\alpha\}$ only, and thus Eq.(60) gives us the series expansion for H_{eff} $(\{Q_\alpha\})$ in powers of $(H_1 + H_2)$. The effective Hamiltonian is seen to be a sum of terms involving many body forces. The nth order cumulant involves at most (n+1) blocks at one time and hence contains at most (n+1) body forces.

We can regroup these terms and separate out the "irreducible" one body interaction, the "irreducible" two body interaction etc. using the following criterion : An irreducible n-body interaction term is nonzero only if each of the charges contributing to the n-body interaction is nonzero.

If an n-body interaction term is not irreducible, it may be written as a sum of an n-body irreducible interaction and fewer body irreducible interactions. For example,

consider a term in the second cumulant which does not satisfy our criterion

$$T = 2 \sum_{\alpha,\beta} \mu_{2,0,0}(Q_\alpha) \quad \mu_{2,0,0}(Q_\beta)[\psi_{11}(\alpha,\beta)]^2 \ . \tag{61}$$

This may be written as

$$T = T_0 + T_1 + T_2 \ , \tag{62}$$

where

$$T_0 = 2 \sum_{\alpha,\beta} \mu_{2,0,0}(0) \quad \mu_{2,0,0}(0)[\psi_{11}(\alpha,\beta)]^2 , \tag{63a}$$

$$T_1 = 4[\sum_{\alpha} \delta\mu_{2,0,0}(Q_\alpha)] \ [\sum_{\beta} \{\psi_{11}(\alpha,\beta)\}^2 \mu_{2,0,0}(0)] , \tag{63b}$$

$$T_2 = 2[\sum_{\alpha,\beta} \delta\mu_{2,0,0}(Q_\alpha) \, \delta\mu_{2,0,0}(Q_\beta)\{\psi_{11}(\alpha,\beta)\}^2] \tag{63c}$$

where we have put

$$\delta\mu_{2,0,0}(Q_\alpha) = \mu_{2,0,0}(Q_\alpha) - \mu_{2,0,0}(0) . \tag{63d}$$

The terms T_0, T_1 and T_2 are clearly irreducible 0-body, irreducible one-body, irreducible 2-body terms. (An irreducible 0-body term in the Hamiltonian is just an additive constant to the Hamiltonian.) We thus write

$$\begin{aligned} H_{eff}(\{Q_\alpha\}) = & -\tilde{A}_c/\beta_{eff} - (1/\beta_{eff}) \sum_{\alpha} \ln\tilde{I}(Q_\alpha) \\ & - (1/2) \sum_{\alpha \neq \beta} \tilde{\Phi}_{QQ}(\alpha-\beta) Q_\alpha Q_\beta \\ & + (1/2) \sum_{\alpha,\beta} \tilde{V}_2(\alpha,Q_\alpha;\beta,Q_\beta) \\ & + (1/3!) \sum_{\alpha,\beta,\gamma} \tilde{V}_3(\alpha,Q_\alpha;\beta,Q_\beta;\gamma,Q_\gamma) \\ & + \text{higher body interactions.} \end{aligned} \tag{64}$$

Here $\widetilde{V}_n$ stands for the n-body irreducible interaction. The advantage of this decomposition is that the effect of the n-body interaction $\widetilde{V}_n$ is now proportional to the nth power of the charge density. For small charge densities, (as will be shown to be the case near the fixed point of the renormalization transformation) the terms with $n \geq 3$ may be neglected.

Note that in Eq.(64) we have two terms involving the two-body interaction. It is useful to separate out the Coulomb interaction between the blocks $\widetilde{\Phi}_{QQ}$, from the "residual" two-body irreducible interaction $\widetilde{V}_2$ which is expected to be small.

Usually, we should be able to determine the irreducible 0-body, 1-body, 2-body ....interactions, by considering the cases when only 0,1,2.... of the charges are nonzero. This is not possible because of the constraint $\sum_\alpha Q_\alpha = 0$. A configuration with only one nonzero charge is not allowed. We are thus free to define the one body potentials any way we like, so long as the corresponding two body interactions are appropriately defined. In particular, the Hamiltonian is unchanged under the transformation

$$\widetilde{\Phi}(R) \longrightarrow \widetilde{\Phi}(R) + c[1 - \delta_{\vec{R},\vec{0}}], \tag{65a}$$

$$\tilde{I}(Q) \longrightarrow \tilde{I}(Q)\exp(c\,\beta_{eff}\,Q^2/2), \tag{65b}$$

for any constant c.

However, once the one and two body potentials are defined, the higher irreducible interactions are defined unambiguously.

It is shown in Appendix D that the potential $\tilde{\Phi}_{QQ}(R)$ varies logarithmically for large R. We have for large R

$$\beta_{eff}\tilde{\Phi}_{QQ}(R) = \beta\Psi_{QQ}(R) - (A\ell nR + B) + c\,\beta_{eff}. \tag{66}$$

Here $(A\ell nR + B)$ is the correction to the Coulomb interaction between blocks due to the polarizability of the surrounding medium. A and B are some constants that go to zero approximately as $[I(1)]^2$. c is an arbitrary constant which we are free to choose [Eq.(65)] Now, we use our freedom to choose the constants β_{eff} and c, so so that the new potential $\tilde{\Phi}_{QQ}(R)$ differs from the original potential $\Phi(R)$ as little as possible. We put

$$\beta_{eff} = \beta - A\pi, \tag{67}$$

and

$$c = B/\beta_{eff} + (\gamma + \tfrac{3}{2}\ell n2)/\pi - \beta(\gamma + \tfrac{5}{2}\ell n2)/\beta_{eff}, \tag{68}$$

so that we have for large R

$$\tilde{\Phi}_{QQ}(R) \approx (1/\pi)\{\ell nR + \gamma + (3/2)\ell n2\} + O(R^{-1}), \tag{69}$$

$$= \Phi(R) + O(R^{-1}). \tag{70}$$

With this choice of β_{eff} and c specified, we now have an explicit computational procedure for determining H_{eff} from H.

Of course, we can repeat the procedure again, and reduce the number of degrees of freedom again by a factor of 4. The many body interaction terms in H_{eff} are included in H_2 . This makes the explicit calculation of cumulants much more difficult, but does not cause any difficulty in principle. We write

$$H_{eff} = \mathcal{R}(H), \tag{71}$$

where $\mathcal{R}$ is the (nonlinear) renormalization transformation operator which maps the Hamiltonian H into the Hamiltonian H_{eff} . The operator $\mathcal{R}$ may be applied more than once. Define

$$H_{eff}^{(r+1)} = \mathcal{R}\,[\,H_{eff}^{(r)}\,]. \tag{72}$$

In the next section we study the asymptotic properties of the sequence of Hamiltonians $H_{eff}^{(r)}$ for large r, and deduce from this the critical behavior of the system.

V : ANALYSIS OF THE RECURSION EQUATIONS

As is perhaps fairly clear by now, the full renormalization transformation is very complicated and difficult to implement. Fortunately we do not need to analyse the full recursion equations in order to determine the critical properties of the model. For this purpose, usually the knowledge of the fixed points of the transformation and the behavior of the transformation near its fixed points is quite sufficient. In the following analysis we shall make many approximations in determining the nature of the phase transition near its critical point. While the approximations may be sometimes quite crude, it should be emphasized that they are unimportant in that they do not change the nature of the phase transition near the critical point. It should be possible, though extremely tedious, to justify each approximation at each step. We shall not make such an attempt, and depend mainly on physical intuition for their justification. The critical behavior is determined <u>exactly</u> in spite of the approximations.

Near the critical point, the recursion equations simplify considerably. As we shall show, charge densities are arbitrarily small if we are sufficiently close to the critical point Hamiltonian. Hence the many body terms $\tilde{V}_n$

in the Hamiltonian ($n \geq 3$) may be ignored. Similarly, the operator $\tilde{V}_2$, though it is a two body operator and hence of the same order in charge densities as the Coulomb interaction term $\tilde{\Phi}_{QQ}$ which we retain, turns out to be an "irrelevant operator" in the jargon of renormalization theory. (Irrelevant operators are those terms in a Hamiltonian whose deviations from their fixed point values decrease on renormalization. Hence after a few iterations of the renormalization transformation, the irrelevant operators are essentially fixed at their fixed point values, irrespective of their starting values. The critical behavior of the Hamiltonian is independent of their precise value.) It can thus be ignored without affecting the critical properties of the model. For further discussion on this point, please see Appendix D.

We need to determine the effect of the renormalization transformation on the Hamiltonian H, when the activities I(Q) of the charges are small for $Q \neq 0$. Since we have decided to ignore the many-body interactions and the $\tilde{V}_2$ interaction, the Hamiltonian is now characterized by the two-body Coulomb potential $\tilde{\Phi}_{QQ}$, the one body potentials $\tilde{I}(Q)$, and the effective temperature β_{eff}. Hence, in this approximation of small charge densities, the recursion equation (71) may be simplified to

$$H[\beta_{eff}, \tilde{\Phi}_{aa}, \tilde{I}(Q)] = \mathcal{R}\, H[\beta, \Phi_{aa}, I(Q)] , \tag{73}$$

which just says that the renormalization transformation maps one set of values $[\beta, \Phi_{aa}, I(Q)]$ to a different set $[\beta_{eff}, \tilde{\Phi}_{aa}, \tilde{I}(Q)]$.

It is easy to identify the fixed points of this transformation. There is a line of fixed points

$$H^* = H^*[\beta^*, \Phi^*, I^*(Q)] , \tag{74}$$

such that

$$\mathcal{R} H^* = H^* . \tag{75}$$

Here the fixed point values of $I^*(Q)$ and Φ^* are given by the equations

$$I^*(Q) = \delta_{Q,0} , \tag{76}$$

$$\Phi^*(\vec{R}) = (1/\pi)[\gamma + (3/2)\ln 2 + \int_{-1/2}^{+1/2}\int dx_1 dx_2 dy_1 dy_2 \ln\{(R_x + x_1 - x_2)^2 + (R_y + y_1 - y_2)^2\}^{1/2}] . \tag{77}$$

and the parameter β^* is arbitrary. That the conditions (76) and (77) lead to a fixed point is easily verified. Eq.(76) makes the activity of any nonzero-charge state zero. Thus the state of the system under H^* corresponds to no charges. Clearly, this state maps onto itself under the renormalization transformation. The potential Φ^* is easily seen to reproduce itself [Eqs.(66-68)] with the choice of the constants

$$A = B = 0, \tag{78a}$$

$$C = -(1/\pi)\ell n 2 . \tag{78b}$$

There is also an isolated fixed point given by

$$\beta^* = 0, \tag{79a}$$

$$I^*(Q) = 1, \text{ for all } Q. \tag{79b}$$

This fixed point corresponds to arbitrarily large densities at different blocks and a complete screening of the Coulomb potential. For this fixed point, the value of the two-body potential Φ^* is clearly unimportant, as it always occurs in the combination $\beta^*\Phi^*$.

Let us now study the stability of the line of fixed points. Consider a starting Hamiltonian with parameters β, $I(Q)$, and $\Phi^*(R) + \delta\Phi(R)$. After one renormalization, these are transformed to (we retain only first order terms in deviations from H^*)

$$\beta' = \beta , \tag{80a}$$

$$I'(Q) = 4\, I(Q) \exp[-\beta Q^2 \ell n 2 /(2\pi)] , \tag{80b}$$

$$\delta'\Phi(\vec{R}) = (1/16) \sum_{\eta_i = \pm\eta_2} \delta\Phi(2\vec{R} + \eta_1 \hat{e}_x - \eta_2 \hat{e}_x + \eta_3 \hat{e}_y - \eta_4 \hat{e}_y) . \tag{80c}$$

Thus we see that if $\beta > 4\pi$, the fixed point Hamiltonian is attractive and successive renormalizations bring the effective Hamiltonian closer to the fixed point.

If $\beta < 4\pi$, the fixed point becomes unstable, because the one-body interaction term I(Q = 1) starts growing with iteration. Successive iterations drive the effective Hamilonian after r iterations, $H_{eff}^{(r)}$, farther and farther away from the fixed point. Eventually, as r tends to infinity, $H_{eff}^{(r)}$ tends to the attractive fixed point given by Eqs.(79a-b).

Consider now the full renormalization transformation given by Eq.(73), when the activities I(Q) are small for nonzero Q. Full here means that we include the effect of nonlinear terms in the transformation (but not the many body interactions). After a small number of iterations of the renormalization transformation, the potential $\tilde{\Phi}(R)$ is fairly indistinguishable from its asymptotic value $\Phi^*(\vec{R})$, and we may replace $\tilde{\Phi}$ by Φ^* in the recursion equations. The recursion equations for I(Q) show that the values of $I_{eff}^{(r)}(Q)$, $|Q| > 1$, are essentially determined by $I_{eff}^{(r)}(Q=1)$, and we have

$$I_{eff}^{(r)}(Q) \approx [I_{eff}^{(r)}(1)]^{|Q|} \; f_Q \; \{1 + \text{terms of order} \left(I_{eff}^{(r)}(1)\right)^2 \}, \quad (81)$$

where f_Q are some absolute constants dependant on Q.

Thus, near the critical point, after a few iterations of the renormalization transformation, a contraction of description takes place and the effective Hamiltonian can be adequately characterized by only <u>two</u> parameters : β_{eff} and $v \overset{def}{=} I(1)$.

It is now easy to write down the recursion equations for these parameters. Remembering that near the critical point, β is close to 4π, and v is close to zero, the renormalization equations take the considerably simpler form

$$\beta^{(r+1)} \cong \beta^{(r)} - K_1 v^{(r)2}, \tag{82a}$$

$$v^{(r+1)} \cong 4v^{(r)} \exp[-\beta^{(r)} \ell n 2/(2\pi)] + K_2 v^{(r)3}, \tag{82b}$$

where we have retained only terms up to the third order in $v^{(r)}$. K_1 and K_2 are some absolute (though lattice dependent) constants whose precise value does not concern us here.

Since the rest of this section is just a detailed analysis of the Eqs.(82), let us pause here a moment to understand these equations physically. $Q_\alpha Q_{\alpha'} \beta_{eff} \Phi_{4\pi}(R)$ measures the effective interaction between any two block charges Q_α and $Q_{\alpha'}$ separated by a distance R. Each block, in addition to the block charge Q, has dipole and quadrupole moments. Thus the charges Q_α and $Q_{\alpha'}$ are in effect immersed in the polarizable medium of other blocks. Hence the effective interaction between them β_{eff}, is <u>less</u> than the bare interaction measured by β. The difference is proportional to the polarizability of the medium, and this is clearly proportional to v^2 for small v.

The recursion equation (82b) for $v^{(r+1)}$ is also easy to understand. The factor 4 comes from the four possible positions of the single charge on the block. The second and the third terms come from the shifting of the two-body potential by an amount c [Eqs.(65) and (68)]. Again the correction due to the polarizability of the medium is proportional to v^2 for small v. We might even say that these equations (82) could be written down from first principles, without having to develop the full formalism of the renormalization transformation.

For small values of $(\beta - 4\pi)$ and v , their values change very slowly with r , and the discrete recursion equations (82) may be profitably approximated by the corresponding differential equations

$$\frac{d\beta}{dr} = -K_1 v^2 \quad , \tag{83a}$$

$$\frac{dv}{dr} = (4\pi - \beta)v \ \ell n 2 /2 + K_2 v^3 \ . \tag{83b}$$

These equations may be solved easily to determine v and β as functions of r. The trajectories of $\beta(r)$ verses v(r) are shown in Fig.14. The trajectories are approximately hyperbolas near $\beta = 4\pi$ and v = 0. They may be parameterized by a single parameter E, and are given by

$$(\beta - 4\pi)^2 = v^2 \, 2K_1 / (\ell n 2) + E. \tag{84}$$

If we fix the starting value of v at v_o , and vary β_o, the parameter E varies according to the Eq.(84). If E =0, we

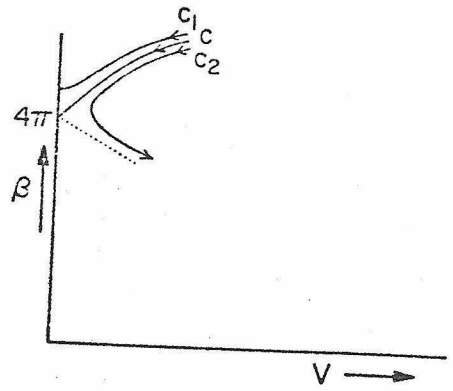


FIG. 14. The trajectories Of $\beta(r)$ vers. v(r). The curve C_1 corresponds to a temperature of the charged gas below the critical temperature. It ends at a fixed point on the v=0 axis. Curve C is the critical curve and ends at the point v=0, $\beta=4\pi$. The curve C_2 is for a charged gas at a temperature above the critical temperature. For large r, it tends towards the point v=1, $\beta=0$ (not shown in the figure) .

get the critical curve C (Fig.14) which ends at the fixed point $\beta=4\pi$, v=0. Clearly the parameter E is linear in the temperature difference $[\beta_c - \beta_c(v_o)]$, if the starting temperature β_o is slightly different from the critical temperature $\beta_c(v_o)$.

If E>0, the starting point is above the curve C in Fig. 14 and the trajectory follows a curve similar to C_1. As r tends to infinity, the curve C_1 tends towards the fixed point $\beta = 4\pi + \sqrt{E}$, v = 0 .

If $E < 0$, the point (β, v) tends initially towards the $v=0$ axis, but is ultimately repelled away from it and tends towards the fixed point $v = 1$, $\beta = 0$. This point is very much to the right of the figure, and is not shown in the figure as the corresponding value of v is large and the small v approximation breaks down.

Substituting the approximation (84) into the Eq.(83a), we get

$$d\beta/dr = -(\ell n 2)\,[(\beta - 4\pi)^2 - E]/2 \qquad (85)$$

The solution of this equation for the case $E > 0$ is

$$\frac{\beta - 4\pi - \sqrt{E}}{\beta - 4\pi + \sqrt{E}} = \frac{\beta_0 - 4\pi - \sqrt{E}}{\beta_0 - 4\pi + \sqrt{E}} \exp[-\ell n 2 \sqrt{E} r] \qquad (86a)$$

If $E = 0$, the solution is

$$(\beta - 4\pi)^{-1} - (\beta_0 - 4\pi)^{-1} = r\,\ell n 2 / 2. \qquad (86b)$$

And if $E < 0$, the solution is

$$\tan^{-1}\left(\frac{\sqrt{|E|}}{\beta - 4\pi}\right) - \tan^{-1}\left(\frac{\sqrt{|E|}}{\beta_0 - 4\pi}\right) = (\ell n 2)\, r\sqrt{|E|}/2 \qquad (86c)$$

In all these equations β_0 is the value of β for $r=0$. $v(r)$ may be obtained by differentiating $\beta(r)$ with respect to r [Eq.(83a)].

We now determine the critical properties of the Coulomb gas from these recursion equations.

Clearly E =0 corresponds to the critical curve separating the low temperature phase of the Coulomb gas where charges form bound pairs (region above the curve C in Fig.14) from the high temperature phase where charges are unbound (region below the curve C in Fig. 14) . If $\beta_c(v_o)$ is the inverse critical temperature corresponding to the activity v_o for unit charges, we have for small v_o

$$\beta_c(v_o) \approx 4\pi + v_o (2K_1 / \ell n 2)^{1/2} \quad . \tag{87}$$

This result is, of course, very plausible and says that if the activities of the charges are increased, the medium is more easily polarized, and the critical temperature for the breakdown of bound charges is decreased.

Let us now consider the constant term $\tilde{A}_o$ generated by the renormalization transformation , which we have ignored so far. This is the term which determines the Landau potential of the system. In fact, the Landau potential per site g, satisfies the exact equation

$$g = \beta_c^{-1} \sum_{r=1}^{\infty} A_o^{(r)} 4^{-r} \quad . \tag{88}$$

Using the approximate expression for $v^{(r)}$ obtained by differentiating Eq.(86) , it is easy to verify that g has an essential singularity as a function of E , and that the singular part varies as $\exp[-K|E|^{-1/2}]$ for small E, where K is some positive constant. Thus we see that the Landau potential g has an essential singularity as a function of

temperature.

As r tends to infinity, the behavior of $\beta(r)$ is quite different above and below the critical point. The limiting value is zero for temperatures above the critical point, and a finite value $\approx(4\pi+\sqrt{E})$ below the critical temperature. As was pointed out earlier, $\beta(r=\infty)$ measures the strength of the effective interaction between two charges very far away from each other, and it follows that $\beta(r=0)/\beta(r=\infty)$ is equal to the dielectric constant of the charged gas. It is finite for temperatures below and at the critical temperature but is infinite above it. Thus we see that the dielectric constant just below the critical temperature is given by

$$\mathcal{E} \approx (\beta_c/4\pi) - K(T_c - T)^{1/2}. \qquad (89)$$

Here again K is a constant of proportionality. We are, of course, working in natural units and T_c is just a number.

Finally, let us determine the behavior of the correlation length as the temperature tends to the critical value from below. The correlation length varies as 2^{r_o} where r_o is the number of iterations of the renormalization transformation needed to reach some preassigned cutoff value of $V_{cutoff}(r)$. Clearly, from Eq.(86a), r varies as $E^{-1/2}$, and hence the correlation length varies as $2^{E^{-1/2}}$.

This concludes our discussion of the critical behavior of the charged lattice gas. These results are easily translated into the language of the melting model. We see that the transition temperature for the melting model is given by [Eq.(15)]

$$k_B T_{c,m} \pi^2 / m_c c^2 = \beta_c = 4\pi + K V_o \ . \qquad (90)$$

Here $T_{c,m}$ is the critical temperature for the melting model and K is some constant of proportionality. The result is valid for small V_o only. Thus the melting temperature increases as V_o is increased. For large values of V_o , the increase in the melting temperature is much slower due to the presence of higher order terms in V_o in Eq.(90). In particular, we expect the melting temperature to remain finite as V_o tends to infinity.

Similar to the singularity of the Landau potential for the charged gas , the free energy and the specific heat for the melting model show only a very weak essential singulatity [$C_v \sim \exp(-K|T-T_{c,m}|^{-1/2})$] as a function of temperature.

The correlation function shows a sharply discontinuous behavior near the critial temperature. The mean squared deviation between the the sites (0,0) and $\vec{R}$ in the melting problem corresponds to effective potential between the same sites for a charged gas. We have, thus, for $T>T_{c,m}$, with

$T-T_{c,m}$ small,

$$\lim_{R\to\infty} \langle (x_{\vec{c}} - x_{\vec{R}})^2 \rangle \, 2\pi^2/(a^2 \ln R) = 4 + K(T - T_{c,m})^{1/2}, \quad \text{for } T \gtrsim T_{c,m}; \tag{91}$$

$$= 0 \qquad \text{, for } T < T_{c,m} . \tag{92}$$

For $T<T_{c,m}$, the mean square deviation does not increase with $|\vec{R}|$ indefinitely. We can easily derive the asymptotic behavior of $\langle (x_{\vec{c}} - x_{\vec{R}})^2 \rangle$ as R tends to infinity. In the charged lattice gas language, this corresponds to evaluating the finite energy needed to create two charges infinitely separated from one another, in the presence of the ionized Coulomb gas at $\beta < \beta_c$. Now, the total interaction energy between two charges Q and Q' infinitely separated from one another is

$$-QQ' \beta_a^{-1} \sum_{r=1}^{\infty} \beta^{(r)} C^{(r)} . \tag{93}$$

The number of iterations needed to change the value of from $4\pi + \sqrt{|E|}$ to $4\pi - \sqrt{|E|}$ is approximately given by Eq.(85c)

$$r_o = \pi / (\ln 2 \, |E|^{\frac{1}{2}}) . \tag{94}$$

For these values of r, the constants $c^{(r)}$ are close to $(1/\pi)\ln 2$. For larger values of r, the function $\beta^{(r)}$ tends very quickly to zero. Hence we have

$$\sum_{r=1}^{\infty} c^{(r)} \beta^{(r)} \approx r_o \ln 2 / \pi = |E|^{-\frac{1}{2}} . \tag{95}$$

But E is proportional to the temperature difference away from the critical point. And thus we find that the mean square deviation increases as $(T_{c,m} - T)^{-1/2}$ in the melting

model as the temperature approaches $T_{c,m}$ from below.

VI : CONCLUDING REMARKS

The treatment in the previous two sections showed that a two dimensional layer in a small external periodic potential undergoes a phase transition at a temperature given by

$$k_B T_c \approx (4/\pi) m_e c^2 \ , \qquad (96)$$

where m_e is the mass of one atom and c is the velocity of sound in the medium. This is, of course, a restatement of the Lindemann's melting criterion, which states that solids melt when the root mean square deviation of an atom reaches a critical fraction of the lattice spacing. Taking a typical example of silver (molecular weight = 108; velocity of transverse sound =1600 m/sec) , we get a prediction of the melting temperature 4.2×10^4 °K. This should be compared with the experimental value T =1233°K. We see that our predicted temperature for melting is about 35 times higher than the experimental value. The agreement looks much more reasonable if, instead of comparing the melting temperature, we compare the value of the fraction $f = \sigma/a$, where σ is the root mean square deviation of atoms in the solid just below the melting temperature, and a is the lattice spacing. For real materials, this value is close to 0.10. In our model the value of this fraction is close to 0.6 .

That our predicted temperature is too high by a factor of about 35, should not cause much concern. In fact, there would be reason to worry if the predicted temperature were closer to the experimental value. This is because our model is highly simplified. In particular, we have introduced anharmonic interaction only between layers. Witnin each layer, the coupling between atoms was assumed to be purely harmonic. Furthermore, the layers adjacent to the layers under discussion were assumed held fixed. If this is not done, the onset of slipping should take place much earlier, because it would be possible to obtain much greater root mean square deviation at lower temperatures by the cooperative action of each layer being slightly displaced with respect to the previous one.

Both of these effects, acting independently, can decrease the transition temperature by a factor of 5 to 10. Also, in some cases, e.g. solid helium, the quantum mechanical zero point energy of vibrations is significant and decreases the transition temperature still further.

While the formal treatment of the model is very similar to the Kosterlitz-Thouless dislocation melting in two dimensions, it must be emphasized that the physical picture is quite different. In the dislocation model, the two dimensional 'charges' correspond to dislocations, whose density increases as the temperature is increased. In our

model, the charges are something like "solidification centers". The density of these "solidification centers" is very small at high temperatures in the liquid phase. The solid phase corresponds to a high density of these charges. Also, as mentioned earlier, the behavior of the dislocation model depends on the lattice structure of the two dimensional lattice, being different for the square and the triangular lattices. Such a situation does not arise in our model and the critical behavior of the model is independent of the lattice structure.

We note that the melting transition in our model is a continuous transition, with no latent heat. This is a major inadequacy of our model, as all the melting transitions occuring in nature are first order. It is however, possible that a first order transition will be obtained if the magnitude of the periodic potential V_o is not assumed constant in the model, but is determined within the model in some self-consistent manner. Physically, such a self-consistency approximation takes into account the decrease in the magnitude of the effective periodic potential due to the random thermal motion of the adjacent layers. We have not succeeded so far in overcoming the mathematical difficulties encountered in the implementation of such an approach. This seems to be a promising area for further investigation.

Our approach to the melting transition differs in one important respect from earlier approaches. Most of the simplifications and approximations of the model are included in the model Hamiltonian. Once the Hamiltonian is written down, we do not make any more ad hoc approximations of dubious validity. The critical behavior is exactly determined for the assumed form of the Hamiltonian.

Also, the model treats the low temperature and the high temperature phases on equal footing. This should be contrasted with other theories of melting, which are essentially one phase theories and only determine the temperature beyond which the theory breaks down. (An example would be a theory that identifies the melting temperature as the temperature beyond which the theory gives a negative value for the shear modulus.) It is also superior to mean field type theories in that it takes into account the fluctuations near the transition temperature (at least in two directions).

The relationship of this model of melting to the melting transition in real materials is, at best, similar to that of a caricature (as opposed to that of a portrait or a hologram) to a person. Some features of reality are very much magnified, while others are completely ignored. The qualitative picture of the melting transition , as it emerges from the model, is presumably correct. A precise

agreement with experiments should not be expected.

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APPENDIX A

We consider the equation

$$F(\lambda) = -[(n-2)/4n]\ell n\,[(\lambda+n)(\lambda+n+2)] + (1/n)F(n\lambda+2\lambda+\lambda^2). \qquad (I\ 11)$$

This equation is valid for all $\lambda > 0$. As λ tends to infinity, $F(\lambda)$ tends to $-(1/2)\ell n\lambda$. This condition specifies $F(\lambda)$ completely, when combined with Eq.(I 11). From Eq.(I 10) we may write

$$F(\lambda) = -(1/2)\int_0^\infty d\omega^2 D(\omega^2)\ \ln(\omega^2+\lambda)\ , \qquad (A1)$$

where $D(\omega^2)d\omega^2$ is the fractional number of modes in the frequency range ω^2 to $\omega^2+d\omega^2$. From Eq.(A1) we may define $F(\lambda)$ as an analytic function of λ over the entire complex λ-plane. The function has logarithmic branch points on the negative real axis and consists of many sheets. Consider the sheet in which $F(\lambda)$ is real for all real positive λ. We make a branch cut along the negative real line. Then it is easy to see that

$$H(\omega^2) \overset{def}{=\!=} -(2/\pi)\,\mathrm{Im}\ F(-\omega^2+i\varepsilon)\ , \text{ for all real } \omega^2, \qquad (A2)$$

$$= \int_0^{\omega^2} d\omega'^2 D(\omega'^2), \text{ for } \omega^2 > 0. \qquad (A3)$$

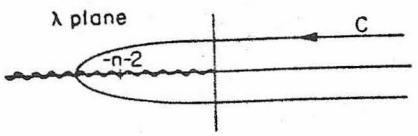


FIG. 15. The complex λ plane showing the curve C and the branch cut along the negative real axis.

Consider $\lambda = \lambda_R + i\epsilon$, where λ_R is real. As we vary λ_R from $+\infty$ to $-\infty$, the function $(n\lambda + 2\lambda + \lambda^2)$ traces out the curve C shown in Fig. (15). For $\lambda_R < -(n+2)/2$ the curve C crosses over the negative real axis and goes into a different sheet. The value of the function $F(\lambda)$ on this sheet differs from its value on the original sheet by an additive imaginary constant. Taking the imaginary part of Eq.(I 11) it is easy to show that

$$H(\omega^2) = (1/n)\, H(n\omega^2 + 2\omega^2 - \omega^4) \quad , \text{ for } 0 < \omega^2 < (n+2)/2, \tag{A4}$$

$$H(\omega^2) = \left[\frac{n-2}{2n} \right] [E(\omega^2 - n) + E(\omega^2 - n - 2)] + (2/n) - (1/n) H(n\omega^2 + 2\omega^2 - \omega^4), \quad \text{for } (n+2)/2 < \omega^2 < \infty, \tag{A5}$$

where $E(x)$ is a unit step function which is zero for negative arguments and +1 for positive arguments. From Eq.(A3), it is easy to see that $H(\omega^2)$ is a non-negative monotonically increasing function of ω^2, and we have

$$H(\omega^2) = 0, \text{ for } -\infty < \omega^2 \leq 0, \tag{A6}$$

$$H(\omega^2) = 1, \text{ for } (n+2) < \omega^2 < \infty. \tag{A7}$$

We shall determine the function $H(\omega^2)$ in the unknown range $0 < \omega^2 < (n+2)$ by repeated applictions of Eqs. (A4) and (A5).

Consider $\omega_1^2 < \omega^2 < n$, where $\omega_1^2(n+2) - \omega_1^4 = n+2$. Then from Eq.(A7), we get $H(n\omega^2 + 2\omega^2 - \omega^4) = 1$; and hence by using Eqs.(A4) and (A5) we get

$$H(\omega^2) = 1/n \text{ , for } \omega_1^2 < \omega^2 < n. \tag{A8}$$

Consider again $n<\omega^2<\omega_2^2$, where $(n+2)\omega_2^2-\omega_2^4=n+2$. Then again $H(n\omega^2+2\omega^2-\omega^4)=1$ by Eq.(A7) , and using Eq.(A5) we get

$$H(\omega^2) = 1/2 \text{ , for } n<\omega^2<\omega_2^2. \tag{A9}$$

Thus we have determined the function $H(\omega^2)$ in the interval $\omega_1^2<\omega^2<\omega_2^2$. This can be used to determine the function $H(\omega^2)$ in the ranges $\omega_3^2<\omega^2<\omega_4^2$ and $\omega_5^2<\omega^2<\omega_6^2$, where ω_3^2, ω_4^2, ω_5^2, ω_6^2 are constants determined by the equations

$$(n+2)\omega_3^2-\omega_3^4=(n+2)\omega_4^2-\omega_6^4=\omega_1^2, \tag{A10}$$

$$(n+2)\omega_4^2-\omega_4^4=(n+2)\omega_5^2-\omega_5^4=\omega_2^2, \tag{A11}$$

and so on. Eventually $H(\omega^2)$ is determined in all the interval $0<\omega^2<(n+2)$, except for some small set of zero measure. Thus we see that $H(\omega^2)$ is constant everywhere except for an infinite but denumerable number of points where its value increases discontinuously. $D(\omega^2)$,which is the derivative of $H(\omega^2)$ and is the spectral density of the system, is a sum of an infinite number of delta functions. Also the points $\omega^2=0$ and $\omega^2=(n+2)$ are clearly points of accumulation of the delta functions and hence again by Eqs. (A4) and (A5) , there are an infinite number of such points of accumulation. Clearly the function $D(\omega^2)$ is a highly singular function of ω^2. However, in thermodynamics, we are

usually interested only in integrals of $D(\omega^2)$ multiplied by some sufficiently smooth function of ω^2. Hence only some sort of smeared value of $D(\omega^2)$ is of interest. It is easy to prove that in this case there exist nonzero finite constants A and B such that

$$H(\omega^2) < A\omega^d, \tag{A12}$$

and $H(\omega^2) > B\omega^d$, for $0<\omega^2<(n+2)$, (A13)

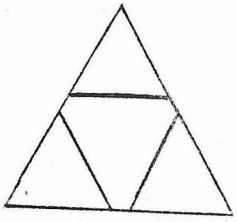
where

$$d = 2\ln(n) / \ln(n+2) . \tag{A14}$$

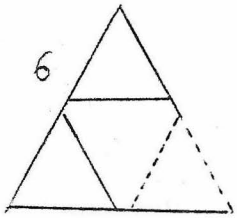
This result is sufficiently strong to permit us to identify d as the effective dimensionality of the lattice.

APPENDIX B

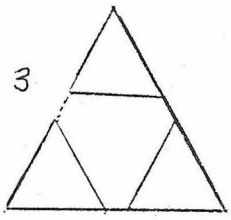
We list here the the configurations and the weights of the r^{th} order triangles that contribute to $Z_3^{(r+1)}$. Contributions to $Z_2^{(r+1)}$ and $Z_1^{(r+1)}$ may be written down similarly. Vertices that are connected together by occupied bonds are shown with a full line joining them. Vertices not connected together by occupied bonds are shown with a dotted line joining them (Eqs. (I 82)).



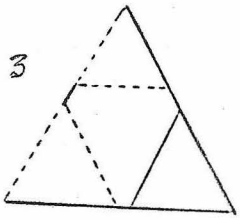
$p^3 K^{-2} Z_3^3$



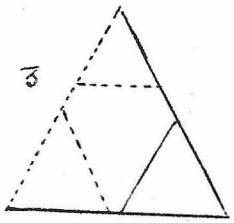
$6p^3 K^{-3} Z_3^2 Z_2$



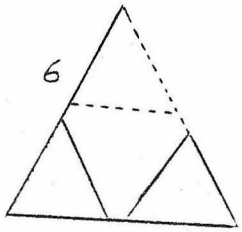
$3p^2 q K^{-2} Z_3^3$



$Z_2^2 3p^3 K^{-3} Z_3$



$3p^2 q K^{-2} Z_3 Z_2^2$

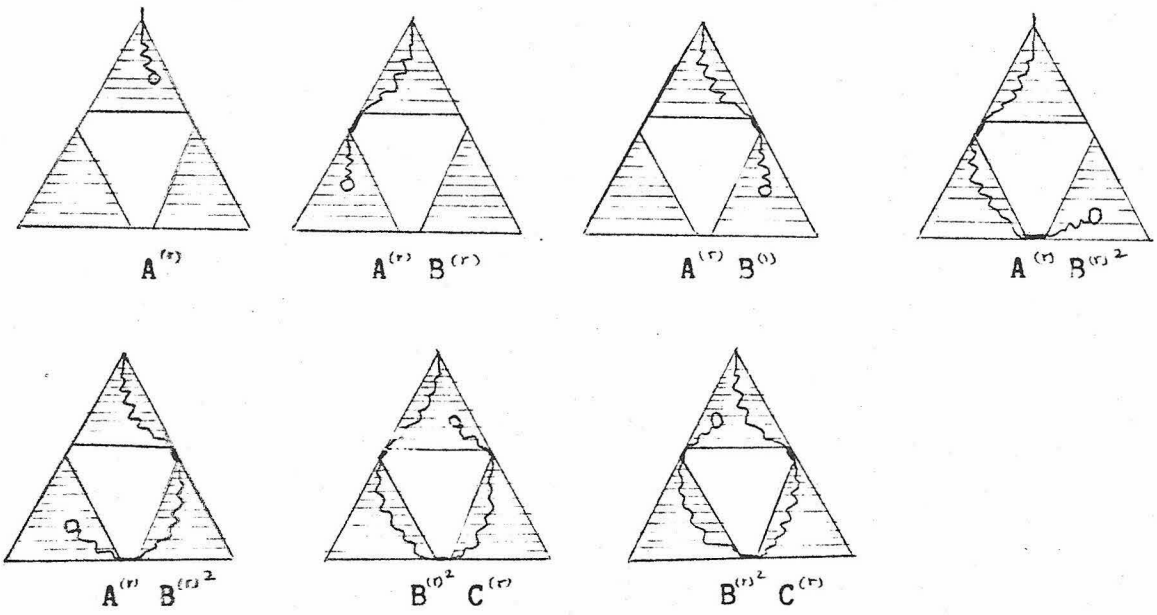


$6p^2 q K^{-2} Z_3^2 Z_2$

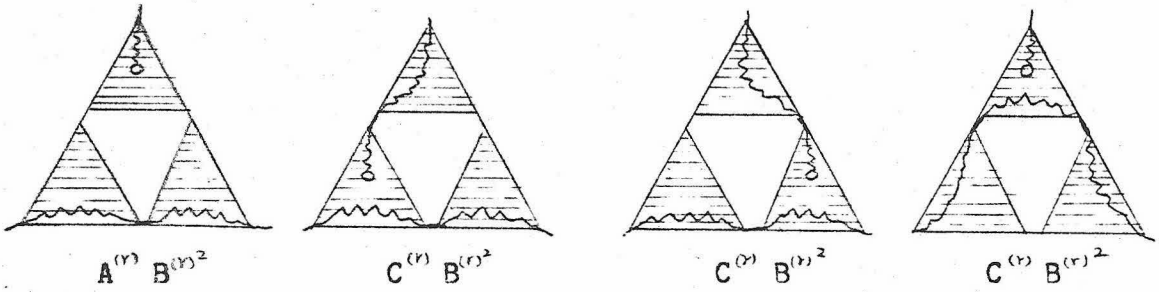
APPENDIX C

We list here all the graphs that contribute to the (r+1)th order vertex-weights for the self-avoiding walk problem on the truncated tetrahedron lattice.

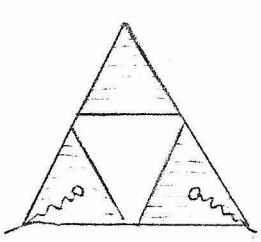
Graphs that contribute to $A^{(r+1)}$:



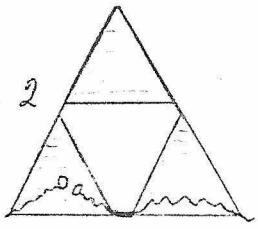
Graphs that contribute to $C^{(r+1)}$:



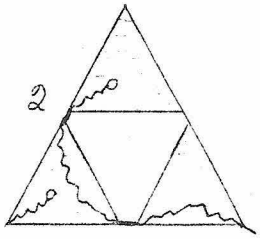
Graphs that contribute to $D^{(r+1)}$:



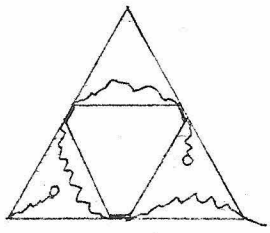
$A^{(r)2}$



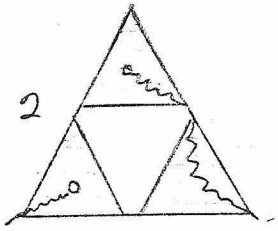
$2D^{(r)}B^{(r)}$



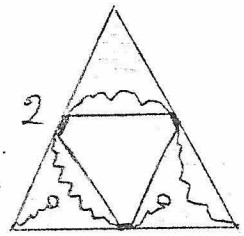
$2A^{(r)}B^{(r)}C^{(r)}$



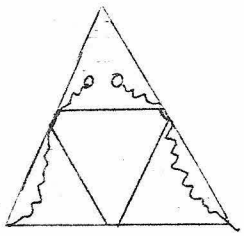
$2C^{(r)2}B^{(r)}$



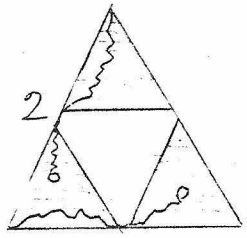
$2A^{(r)2}B^{(r)}$



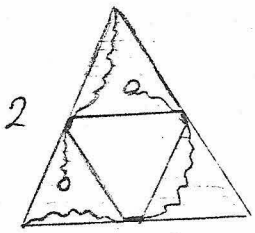
$2C^{(r)2}B^{(r)}$



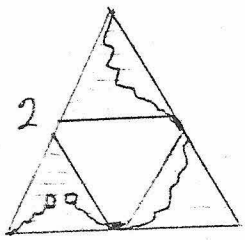
$B^{(r)2}D^{(r)}$



$2A^{(r)}B^{(r)}C^{(r)}$



$2C^{(r)2}B^{(r)}$



$2D^{(r)}B^{(r)2}$

APPENDIX D

We show here that the effective two body Coulomb potential $\widetilde{\Phi}_{qq}(R)$ generated by the renormalization transformation varies logarithmically for large R. The potential $\widetilde{\Phi}_{qq}(R)$ is defined by the Eq.(II64). It is the two body interaction term in H_{eff} which is bilinear in the block charges $\{Q_\alpha\}$. Quite clearly, this can only arise only out of terms that are of second order in the perturbation H_1, though they may contain arbitrary powers of H_2.

In practice, of course, we retain only a finite number of powers of H_2 when evaluating $\widetilde{\Phi}_{qq}(R)$. But for theoretical discussion it is convenient to include the effect of all powers of H_2 by considering a perturbation expansion in powers of H_1 about the unperturbed Hamiltonian $H_o + H_2$. Then clearly the second cumulant of H_1 is given by

$$(\beta^2/2) \sum_{\alpha,\beta,\gamma,\delta} \sum_{p,q=1}^{3} Q_\alpha Q_\gamma \Gamma_{pq}(\beta,\delta)\, \psi_{ap}(\alpha,\beta)\, \psi_{aq}(\gamma,\delta) \quad , \qquad (D1)$$

where we define

$$\Gamma_{pq}(\beta,\delta) = \langle S_{\beta,p}\ S_{\delta,q} \rangle_{H_o+H_2,\{0\}} \, . \qquad (D2)$$

$\Gamma_{pq}(\beta,\delta)$ is the correlation function for the variables $S_{\beta,p}$ and $S_{\delta,q}$ when the Hamiltonian (unperturbed by H_1) is $H_o + H_2$, and all the block charges $\{Q_\alpha\}$ are held fixed at zero values. If the unperturbed Hamiltonian were H_o, the variables $S_{\alpha,p}$ at different blocks would be independent and

we would have

$$\Gamma_{pq}(\beta,\delta) = \Gamma_{pp}(0,0)\,\delta_{\beta,\varepsilon}\,\delta_{pq} \quad . \tag{D3}$$

This is not the case in the presence of H_2, which explicitly couples the $S_{\alpha,p}$ variables at different sites. However, these couplings are weak and they die off at large separations at least as fast as R^{-2}. Furthermore, they tend to cancel each other on the average, as the potentials Ψ_{pq} are as often positive as negative. We thus expect that

$$\Gamma_{pq} \overset{def}{=} \sum_{\beta}\Gamma_{pq}(0,\beta) \tag{D4}$$

exists and is finite. Also $\Gamma_{pq}(\beta,\delta)$ should decrease for large separations at least as fast as $|\beta-\delta|$. The summation in the expression (D1) may be simplified by a Fourier transformation. We get

$$\sum_{p,q=1}^{3}(\beta^2/2)\int\frac{d^2\bar{k}}{(2\pi)^2}\,Q(\bar{k})Q(-\bar{k})\,\Gamma_{pq}(\bar{k})\,\Psi_{Qp}(\bar{k})\,\Psi_{Qq}(\bar{k}) \quad . \tag{D5}$$

Now, $\Gamma_{pq}(k)$ tends to a finite value as $|k|$ tends to zero, and $\Psi_{Q_1}(\bar{k})$ and $\Psi_{Q_2}(\bar{k})$ vary as (k_x/k^2) and (k_y/k^2) respectively for small $|\vec{k}|$. Thus clearly the integrand varies as $Q(\bar{k})Q(-\bar{k})/k^2$ for small $|\vec{k}|$. This implies a logarithmic interaction between the charges $\{Q_\alpha\}$ for large separations. This logarithmic interaction adds to the bare (unperturbed) interaction between the charges $\{Q_\alpha\}$ which is also logarithmic for large separations. We note that magnitude of correction to the bare interaction is proportional to $\Gamma_{11} = \Gamma_{22}$, which is easily seen to be proportional to v^2 for

small v.

APPENDIX E

In this appendix we show that the residual two body irreducible interaction $\widetilde{V}_2$ is an irrelevant operator. We have seen that even if the initial Hamiltonian H does not have any two-body non-Coulomblike interaction terms, these are generated by the renormalization transformation. This raises the possibility that on further iterations of the renormalization transformation, these terms get larger and larger, and thus invalidate our analysis where we have ignored them altogether. We show that this does not happen.

The irreducible two-body residual interaction consists of terms like T_2 [Eq.(II 63c)]. Let us see how this term transforms under the renormalization transformation. We show below that it does not increase without bounds and tends to a finite asymptotic value. Other terms that contribute to the $\widetilde{V}_2$ interaction may be treated similarly. The argument may be generalized to higher body irreducible interactions. We recall that

$$T_2 = 2 \sum_{\alpha\beta} \delta\mu_{2,0,0}(Q_\alpha)\, \delta\mu_{2,0,0}(Q_\beta)[\Psi_{11}(\alpha,\beta)]^2 \ . \qquad \text{(II 63c)}$$

The most important contribution to T_2 comes from the mutual interaction of blocks with block-charges $Q_\alpha = \pm 1$. Near the critical point, higher values of Q_α occur with much lower probability, and in any case, can be treated similarly. If v is small, we have from the defining equation (II 57)

$$\mu_{2,0,0}(\pm 1) = 1 + \text{terms of order } v^2 . \qquad (E1)$$

Let us for the moment neglect other many body interactions and consider the Hamiltonian

$$\beta_{eff}^{(1)} H_{eff}^{(1)} = -\sum_{\alpha} \ell n \tilde{I}^{(1)}(Q_\alpha) - (\beta_{eH}^{(1)}/2) \sum_{\alpha \neq \beta} Q_\alpha Q_\beta \tilde{\Phi}_{\delta\delta}^{(1)}(\alpha,\beta) + T_2^{(1)} . \qquad (E2)$$

Here the superscripts denote the number of iterations of the renormalization transformation. After one more renormalization , this Hamiltonian transforms to

$$\beta_{eff}^{(2)} H_{eff}^{(2)} = A_0^{(2)} - \sum_{\alpha} \ell n \tilde{I}^{(2)}(Q_\alpha) - (\beta_{eH}^{(2)}/2) \sum_{\alpha \neq \beta} Q_\alpha Q_\beta \tilde{\Phi}_{\delta\delta}^{(2)}(\alpha,\beta) + T_2^{(2)} + (\text{n body terms with } n>2). \qquad (E3)$$

The additional terms introduced in the cumulant expansion of $H_{eH}^{(2)}$ due to the presence of $T_2^{(1)}$ in $H_{eH}^{(1)}$ are of the following types :

(i) An additional contribution to the zero body term $A_0^{(2)}$ of order v^2 . This arises due to the configuration of first order block charges ± 1 , lying on the same second order block. Clearly since the second order block has net charge zero, the nonvanishing interaction $T_2^{(1)}$ between these charges will be transformed into a zero-body interaction in $H_{eH}^{(2)}$.

The weight of such configurations is proportional to v^2 , for small v, and hence the correction to the $A_0^{(2)}$ term is of order v^2. Since the only fact about A_0 used in our determination of the critical behavior of the free energy was that A_0 is of order v^2 [Eq. (II 88)], clearly this does not affect our analysis.

(ii) An additional contribution to the one-body terms

$\tilde{I}^{(2)}(Q_\alpha)$. This arises because the weights of internal configurations of a second order block corresponding to a fixed second order block charge Q_α are altered in the presence of the $T_2^{(1)}$ interaction.

If $|Q_\alpha|=1$, such a contribution is of order v^3, because $T_2^{(1)}$ is zero if only one of the first order block charges is zero. All other configurations corresponding to the second order block charge $Q_\alpha = \pm 1$ have weights at least of order v^3.

If $|Q_\alpha| > 1$, the correction term modifies the weights by a finite multiplicative factor. But then $\tilde{I}^{(1)}(Q)$ is itself of order $v^{|Q|}$, and the corrections are of the same order.

As a result, the effect of the term $T_2^{(1)}$ on the recursion equation for v can be absorbed by a change in the value of the constant K_2 in Eq.(II 82b). Again, the critical behavior is independent of the precise value of K_2.

(iii) An additional contribution to the two-body irreducible interaction $T_2^{(2)}$. To the first order in $T_2^{(1)}$, this is just the average value of the mutual interaction $T_2^{(1)}$ between the first order blocks constituting the second order block. We write

$$\delta T_2^{(2)} = \langle T_2^{(1)} \rangle_{H_{0\,eff}^{(1)}}, \qquad (E4)$$

where in obvious notation, $\delta T_2^{(2)}$ is the change in the interaction $T_2^{(2)}$ due to the presence of $T_2^{(1)}$ in $H_{eff}^{(1)}$, and we break up the effective Hamiltonian after one iteration $H_{eff}^{(1)}$ into three terms $H_{0\,eff}^{(1)}$, $H_{1\,eff}^{(1)}$ and $H_{2\,eff}^{(1)}$ as in Eq.(II 44).

Thus, this contribution to the interaction $T_2^{(2)}$, say between second order blocks α and β at a distance $R = |\alpha-\beta|$, is a sort of average value of the interaction $T_2^{(1)}$ between first order blocks at a distance 2R.

If v is small, $H_{0\,eff}^{(1)}$ is very close to $H_{0\,eff}^{(0)}$, and this would be approximately equal to the irreducible two-body residual interaction $T_2^{(0)}$ at a distance 2R. But the interaction T_2 decreases with distance as R^{-4}. [This is obvious from the fact that T_2 varies as $\{\psi_a(R)\}^2$.] Thus we see that (writing $\tilde{V}_2$ instead of T_2 in an obvious generalization)

$$\delta\tilde{V}_2^{(2)}(\alpha,Q_\alpha;\beta,Q_\beta) \approx (1/16)\tilde{V}_2^{(1)}(\alpha,Q_\alpha;\beta,Q_\beta) . \qquad (E5)$$

In addition, the full recursion equations for $\tilde{V}_2^{(2)}$ also include terms generated by the renormalization transformation, even in the absence of the interaction $\tilde{V}_1^{(1)}$ in $H_{eff}^{(1)}$. Hence the recursion equation has the form

$$\tilde{V}_2^{(2)}(\alpha,Q_\alpha;\beta,Q_\beta) \approx (1/16)\tilde{V}_2^{(1)}(\alpha,Q_\alpha;\beta,Q_\beta) + [\text{terms depending on } H_{0\,eff}^{(1)}] + \text{higher order terms.} \qquad (E6)$$

In the jargon of renormalization theory, we say that $\tilde{V}_2^{(2)}$ is a "driven" interaction, in the sense that its value under recursion is primarily determined by interaction parameters in $H_{0\,eff}^{(1)}$, and not so much on $\tilde{V}_2^{(1)}$. In particular, it cannot grow appreciably large unless the contribution to it from $H_{0\,eff}^{(1)}$ becomes appreciable. But this contribution is

of order v^2 , for small v. Hence the neglect of $\widetilde{V}_2$ in the recursion equations is justified and does not affect the critical behavior.

In addition to these terms, $\widetilde{V}_2^{(2)}$ will also contain terms generated by the n-body (n>2) interaction terms in $H_{eff}^{(1)}$. These terms involve higher powers of charge density than two, and hence may be ignored near the critical point.

In the above dicussion, we have avoided writing down explicit expressions for the various terms involved lest the physical argument be lost in the confusion of notation.