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The Use of Reflection as Symmetry Operation in Connection with Peierls' Argument

Ole J. Heilmann
Department of Chemistry, H. C. Ørsted Institute, Copenhagen, Denmark

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Abstract. It is shown that Peierls' argument can be extended to prove the coexistence of states which can be transformed into each other only by reflection, inversion or rotation. This makes Peierls' argument applicable to the repulsive lattice gas on a large class of lattices, as well as many models for liquid crystals, ferroelectrics etc. It is specifiquely shown how the argument can be applied to a lattice gas with nearest neighbour repulsion on the hexagonal lattice and the diamond lattice.

I. Introduction

The Peierls' argument is one of the few methods for proving the existence of phase transition without explicit calculation. The idea goes back to Peierls [1] and the method was given a rigorous formulation for the ordinary, ferro magnetic Ising model by Griffiths [2] and Dobrushin [3]. The argument has later been extended to other lattice models with similar properties [4] and more recently Ruelle [5] has succeeded in applying the method in the first rigorous proof of the existence of a phase transition in a continuous model.

The first application of Peierls' argument to lattice gases with repulsive potential is due to Dobrushin [6] who proved the existence of a phase transition for a lattice gas with nearest neighbour exclusion or nearest neighbour repulsion on a simple cubuc lattice in ν dimensions ($\nu \geqq 2$). The nature of the argument in the case of repulsion is somewhat different from the proof for systems with attractive forces. First, for the ferro magnetic Ising model one utilizes the symmetry between spin-up states and spin-down states in zero magnetic field at the crucial point of the proof; this makes the generalization from simple cubic lattices to any other lattice trivial. For the antiferromagnet one uses a spatial symmetry operation (see below) which is dependent on the structure of the lattice; therefore, this method is not generally applicabel and it should not be so since it is known that if the lattice is

the line graph of another lattice then the antiferromagnet does not have any phase transition [7]. Second, in the case of the repulsive lattice gas one locates an area (in the space of the thermodynamic variables) where the ordered, "crystaline" phase exists with certainty, while one for the attractive gas locates the boundary between two different phases. This has to do with the fact that the "crystalline" phase can exist in several different states which are identical except for a translation or a rotation of the space (real space), and that one proves coexistence of these different states, rather than proving coexistence of really different phase as for the attractive gas.

Dobrushin's proof for the simple cubic lattice uses two properties of the lattice: that it has an A-B-sublattice structure (i.e. the vertices can be divided in two groups (sublattices) such that the neighbours of the vertices in one sublattice always belong to the other sublattice) and that by a translation of one lattice unit the sublattices are interchanged while the lattice is mapped on itself. This makes the proof immediately applicable to the body-centered cubic lattice, but not the triangular lattice which divides into three sublattice or to the hexagonal lattice where one will have to apply rotation, reflexion or inversion to map the lattice on itself in such a manner that the sublattices are interchanged.

Recently, Heilmann [8] and Heilmann and Præstgaard [9] have shown how to overcome the difficulties occuring in the case of three or more sublattices if each of the sublattices can be mapped into any of the other sublattices by a translation which maps the lattice into itself. (In [8] it was incorrectly claimed that this method also applied to the face centred cubic lattice.)

It is the purpose of the present article to complete the investigation of the applicability of spatial symmetry transformation in connection with Peierls' argument by showing how to use reflection, inversion and rotation. The constructions in this cases become vastly more complicated and the reader not interested in technical details is advised to skip the second half of Section 2 (from Condition 2.2) and all of Section 3. The first half of Section 2 contains an outline of the method in very general terms. Section 4 describes the application to the repulsive lattice gas on the hexagonal lattice and the diamond lattice. Section 5 gives a generalization of the results in Section 2 and 3. Finally, Section 6 tries to summarize the models which by the presently known technique can be proved to have a phase transition.

It shall be assumed that the reader is familiar with the Peierls' argument (descriptions can be found to example in Section 2 of [9] and in the review article by Griffiths [10]).

2. The Construction

Let us assume a given lattice model with the following properties given:

1) *Two possible local structures (called A-structure and B-structure) and a definition of how to draw contours between the two structures.* When, in the following, we talk about lattice translation we always mean translations which map A-structure onto A-structure and B-structure onto B-structure.

2) *A configuration should be specified uniquely by specifying all the contours. It should be possible to associate with each contour an energy, such that the energy of a configuration is given as the sum of the energies of the contours. The energy associated with a given contour should be independent of the presence of other contours, but the energy is allowed to depend on which structure is on the inside and which is on the outside. It is assumed that there exists a lower bound on the energy of a contour, which is proportional to the length of the contour.*

3) *There should exist a reflection which maps the lattice (and the model) onto itself while interchanging the two local structures.* The translational invariance will then necessarily imply the existence of a whole system of parallel lines of reflection with a spacing corresponding to the minimum translation which maps the lattice onto itself without interchanging the two local structures. When, in the following, we talk about reflection lines we shall always mean lines taken from this system of parallel lines (i.e. we are not interested in other possible directions).

In the following we will consider a definite contour C which we shall assume to have A-structure on the outside and B-structure on the inside, and we will be interested in making a correspondence between configurations containing C and configurations without C. In this connection the following contours will play a special role:

Definition 2.1. If C is a contour, then a contour is said to be C-1-inner if it is inside C, but not inside any contour which is itself inside C. The set of all C-1-inner contours is denoted $\mathcal{I}(C)$.

One could think of several ways in which to transform a configuration with C into a configuration without C:

a) *One could reflect the configuration inside C in a reflection line.* This would cause a conflict when points inside C were mapped on points outside C. Even with optimal choice of the reflection line the number of such points will in general grow as the area inside C and not as the length of C; therefore, this is too primitive.

b) *One could remove C and all members of* $\mathcal{I}(C)$. This would not cause conflict of structure, but the bound on the loss of entropy will grow too fast, so this does not work either.

c) One could divide the interior of C into regions, each of which could be mapped onto itself by a reflection. This would work if no C-1-inner contour belonged to more than one region. However, even if one let the divisions into regions depend on $\mathscr{I}(C)$, it will in general not be possible to find a proper division.

d) *One could try to combine b and c; i.e. remove some members of* $\mathscr{I}(C)$ *and divide the remaining part of the interior into regions which are invariant under a reflection.* This is the method we shall pursue in the following. First we describe a method for finding the members of $\mathscr{I}(C)$ which should be removed and the regions which can be reflected. Afterwards we demonstrate how this construction can be used to furnish a useful upper bound on the probability of the contour C.

As a first step, we associate with each member of $\mathscr{I}(C)$ a line of reflection. It is important that the definition fulfills the following properties:

Condition 2.2. The reflection line of a contour shall be a proper reflection line (in terms of Condition 3 on the model). The reflection line shall cross (or touch) the contour. The position of the line relative to the contour shall be invariant under lattice translation and reflection in the reflection lines.

The existence of definitions which fulfill Condition 2.2 is not difficult to demonstrate. One could, for example, choose the reflection line as close as possible to the "center of gravity" of the contour, and build in a solution of ambuiguities which agrees with the last sentence of the condition. In general the spacing of the reflection lines will be small enough to ensure crossing; but it might be necessary either to define "touch" in a slight broader sense than normally or to draw the contours appropriately in order to assure at least touching in all cases.

For a given configuration with the contour C we want to find a division of the members of $\mathscr{I}(C)$ into two sets:

Those which are removed with C and those which are reflected in some reflection line. We shall denote the last set by K and use T^* for $\{C\} \cup \mathscr{I}(C) \backslash K$. If the division is correct then we can find a set $\mathscr{M}$ of non-overlapping regions; with each region in $\mathscr{M}$ should be associated a reflection line such that reflection in this line maps the region onto itself. Each member of K should be totally inside a member of $\mathscr{M}$. Preferably, the regions in $\mathscr{M}$ should not overlap with any part of T; however, this turns out to be too restrictive, and we shall therefore in the end of this section modify the argument to allow a C-1-inner contour in T to be totally inside a region in $\mathscr{M}$. During this modification we shall include contours inside C-1-inner contours in the T-contour; thus the final set T of contours to be removed will include C and contours inside C.

We shall obtain $\mathscr{M}$ by starting with an imperfect set $\mathscr{M}_0$, which we then improve step by step until we finally end up with $\mathscr{M}$; simultaneously we find which members of $\mathscr{I}(C)$ should be included in T. At the end of the i'th step T_i will contain the contours which at that stage we have decided to remove, while K_i will contain the remaining members of $\mathscr{I}(C)$. $\mathscr{M}_i$ will be a set of regions which fulfill the following conditions: to each region is associated a reflection line, such that reflection in this line maps the region onto itself; each region is connected and each member of K_i is associated with a member of $\mathscr{M}_i$ which it is totally inside. I.e. the set $\mathscr{M}_i$ has the right properties except that it does not fulfill the overlap condition. One naturally starts with:

Definition 2.3. $T_0 = \{C\}$, $K_0 = \mathscr{I}(C)$. To each member in $\mathscr{I}(C)$ corresponds a member of $\mathscr{M}_0$. The reflection line is the same for corresponding members of $\mathscr{I}(C)$ and $\mathscr{M}_0$; a region in $\mathscr{M}_0$ is obtained from a contour in $\mathscr{I}(C)$ by reflecting the contour in its reflection line and taking the union of the interior of the contour and the interior of the mirror image.

It is easily checked that the $\mathscr{M}_0$ defined above fulfills the conditions we wanted $\mathscr{M}_i$ to fulfill.

In order to describe the process and also afterwards be able to uncover the history of how T was created we need to introduce certain auxiliary concepts describing the structure of the regions in $\mathscr{M}_i$. When we start on the purification process these concepts will only be defined with respect to the initial set $\mathscr{M}_0$. At the i'th step of the purification we shall use the concepts in relation to $\mathscr{M}_{i-1}$ and define them for $\mathscr{M}_i$.

The primary key to the history of the members of $\mathscr{M}_i$, will be a hierarchy of trees[1]. With each member of $\mathscr{M}_i$ we shall associate a tree. The vertices, except the roots of the trees, will themselves represent linear trees, which will be part of trees created earlier; such a linear tree will in the simplest cases contain only one vertex, the root.

The root of a tree will represent a member of K_i (i.e. a C-1-inner contour). The reflection line of a region will be the reflection line of the root (i.e. the reflection line of the C-1-inner contour represented by the root). This is consistent with the following definition for the trees associated with members of $\mathscr{M}_0$.

Definition 2.4. To each member of $\mathscr{M}_0$ is associated a tree with one vertex, the root, which represents the corresponding C-1-inner contour.

When we at the i'th stage look at the trees corresponding to the members of $\mathscr{M}_i$ much of the hisotry of the creation will be burried in the structure inside the vertices (i.e. in the trees represented by the

[1] A tree is a directed graph with one special vertex, the root, which has the property that there is a unique path from the root to any other vertex.

vertices). Most of this structure we will not need for the continuation of the process of purification of $\mathscr{M}_i$ towards the ultimate stage, $\mathscr{M}$. However, one part is needed, and for this we introduce the concept of "a C-1-inner contour being *associated* with a vertex in tree". We shall use a recursive definition, i.e. the full meaning will first appear during the purification process.

Definition 2.5. With a root in a tree is associated the corresponding C-1-inner contour. If η is a vertex representing a tree, τ, then a C-1-inner contour is associated with η if it is associated with a vertex in τ.

During the purification process each member of K_i will be associated with a vertex in a tree in $\mathscr{M}_i$.

The next concept we shall need will be two kinds of auxiliary contours, *R-contours* and *S-contours.* With each vertex in a tree shall be associated an R-contour and an S-contour. They will be built up during the purification process. We start by:

Definition 2.6. For a root both the R-contour and the S-contour are given as the union of the corresponding C-1-inner contour and its mirror image.

When we talk about the S-contour of a tree we shall mean the union of the S-contours of the vertices in the tree. The outer part of the S-contour of tree associated with a member of $\mathscr{M}_i$ will be the boundary of the region. The R-contour of vertex which is not a root will turn out to be the S-contour of the tree represented by the vertex.

We shall further associate two numbers with a vertex, *the reflection number* and *the total s-length.* It will turn out that the S-contour of a vertex is created by reflection from its R-contour. If p is the reflection number of a vertex, then the S-contour will consist of 2^p images of the R-contour. For a root we consequently take the reflection number to be zero. For all other vertices we will find $p \geqq 1$. The other number we define by:

Definition 2.7. With each vertex in a tree is associated a number, t, called the total s-length. It is equal to the sum of the length of the S-contours of vertices on the path from the root to the vertex in question including both the root and the vertex in question.

Remark, that if out of a tree one takes the linear tree from the root to some vertex in the tree then the length of the S-contour of that linear tree is equal to the total s-length, t, for the vertex.

Finally, in order to make the construction unique we need an ordering:

Definition 2.8. The members of $\mathscr{I}(C)$ are ordered by the length of the contours, with the longest first. C-1-inner contours of the same length are ordered primarely by shape and orientation, secondarily by

x-coordinate (with x-axis parallel to the reflection lines) and as last resort by y-coordinate (y-axis orthogonal to x-axis).

Definition 2.9. $\mathcal{N}_i$ is the set of vertices in the trees associated with the members of $\mathcal{M}_i$. The members of $\mathcal{N}_i$ are ordered by their total s-length, t, with the longest first; vertices which have the same total s-length and belong to different trees are ordered by ordering the trees. The trees are ordered by applying the ordering introduced in Definition 2.8 to the roots of the trees. We do not need an ordering for vertices with the same total s-length if they occur in the same tree. [The ordering of $\mathcal{N}_0$ is seen to be the same as the ordering of $\mathcal{I}(C)$].

We can now define the purification process by defining the i'th step.

Definition 2.10. The i'th step in the purification process consist of three substeps (compare Figs. 1–4):

a) The S-contour of each of the members of $\mathcal{N}_{i-1}$ is checked for crossing with T_{i-1}. The members of $\mathcal{N}_{i-1}$ are checked in the order given in Definition 2.9. Suppose the first crossing occurs with the S-contour of the vertex η in the tree τ; the part of τ from the root out to and including η constitutes a linear tree, ω. K_i will then consist of K_{i-1} minus the C-1-inner contours associated with ω, and T_i is obtained by adding these C-1-inner contours to T_{i-1}; $\mathcal{M}_i$ is generated from K_i the same way as $\mathcal{M}_0$ was from K_0 (i.e. the members of $\mathcal{M}_i$ are trees with only one vertex, the root; to each C-1-inner contour in K_i corresponds a member of $\mathcal{M}_i$). As soon as one crossing has been detected and handled the i'th

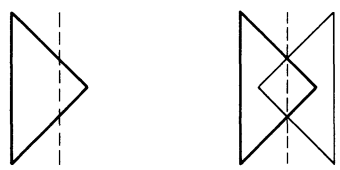

Fig. 1. The figure shows a C-1-inner contour with its reflectionline (left) and the corresponding R-contour (S-contour) after Definition 2.6 (right)

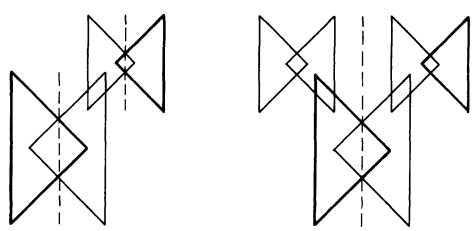

Fig. 2. The figure shows two C-1-inner contours who's S-contours cross (left). To right the S-contour and reflectionline of the resulting tree is shown

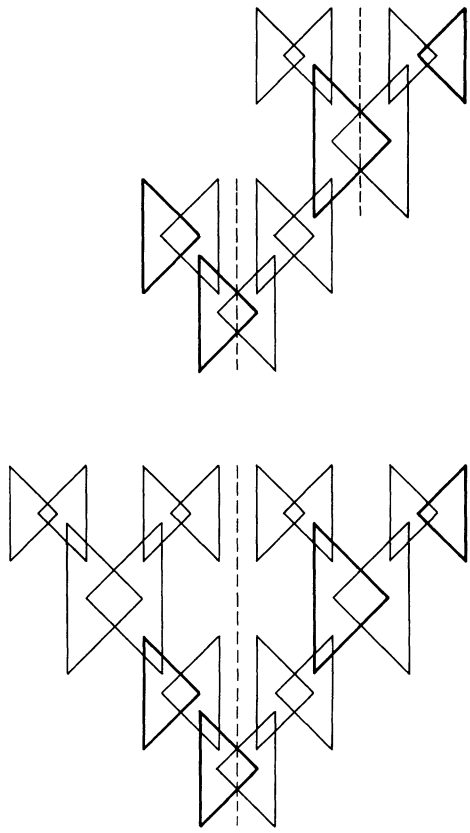

Fig. 3. The figure shows two regions in $\mathcal{M}_{i-1}$ (each containing two C-1-inner contours) who's S-contours cross (top). Below the S-contour and reflectionline of the resulting region in $\mathcal{M}_i$ is shown; the new tree has four vertices

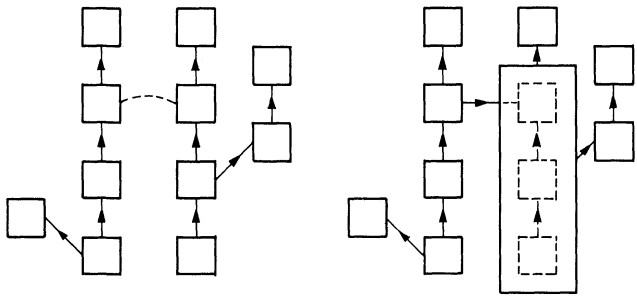

Fig. 4. The figure shows two trees (left) with vertices marked by squares and the edges directed away from the root. The S-contours corresponding to two vertices cross (marked with dotted line), and as a result a new tree is created (right)

step is terminated. If no crossing with the contours in T_{i-1} is found then $K_i = K_{i-1}$, $T_i = T_{i-1}$.

b) The S-contour of each of the members of $\mathcal{N}_{i-1}$ is checked for crossing with the S-contour of any other member of $\mathcal{N}_{i-1}$. The members of $\mathcal{N}_{i-1}$ are checked in the order given in Definition 2.9, and one only checks for crossing between vertices occuring in different trees. Suppose the first crossing is found between S-contours of the vertex η_1 in the tree τ_1 and the vertex η_2 in the tree τ_2; suppose also that η_1 comes before η_2 in the ordering of $\mathcal{N}_{i-1}$. $\mathcal{M}_i$ will then consist of the same regions (and trees) as $\mathcal{M}_{i-1}$ except that the two regions associated with τ_1 and τ_2 are combined into one region. The corresponding tree for that region, τ, is obtained by adding τ_2 to τ_1 in the following manner: The part of τ_2 from the root out to and including η_2 makes a linear tree, ω. In τ, ω is represented by one vertex, η; η is connected by an edge from η_1 to η. The R-contour of η is the S-contour of ω; the S-contour of η is the union of the R-contour and its mirror-image obtained by reflecting it in the reflection line of τ_1. The reflection number of η is 1. The remaining vertices in τ_2 also occur as vertices in τ but their reflection number is increased by 1 and the S-contour is enlarged by taking both the S-contour which the vertex had as a vertex in τ_2 and the mirror image of this contour with respect to reflection in the reflection line of τ_1 (it is possible that during these reflections one creates new S-contour of a vertex on top of its original S-contour; this will amount to some double counting of S-contour, a fact which will not cause any trouble). The edges in this part of τ_2 are kept as edges in τ, except that edges which in τ_2 came from vertices in ω in τ occur as edges from η. As soon as one crossing has been detected and handled the i'th step is terminated.

c) If no crossing has been found under a) and b) then the process is finished. K is equal to K_i. $\mathcal{M}$ is created from $\mathcal{M}_{i-1}$ by deleting the regions which are totally inside another region. The set T^* is equal to T_i.

We can now see the meaning of the edges in the trees. If an edge goes from the vertex η_1 to vertex η_2, and if η_2 represent the linear tree ω, then there is a crossing between the S-contour of η_1 and the S-contour of the last vertex in ω. One also notes that we have defined the S-contour and the reflection number of general vertices. It is worthwhile observing that the process terminates after a finite number of steps.

The S-contour of a tree is, by construction, connected and invariant under reflection in the reflection line of the tree. It is therefore clear that the regions in $\mathcal{M}_i$ have the same properties. Since C is part of T^* and the S-contour is connected, then step a in Definition 2.10 ensures that all the regions in $\mathcal{M}$ are totally inside C; the connecteness also

ensures that the steps b and c together are sufficient to make the regions in $\mathcal{M}$ non-overlaping. The only thing that can go wrong is that one of the C-1-inner contours in T^* ends up totally inside one of the regions in $\mathcal{M}$. Suppose D is such a contour. We then reflect it because it is in a region in $\mathcal{M}$ and when we then have to remove it because it is part of T^* we treat it as we have treated C. I.e. we divide the D-1-inner contours in two groups, one to be removed and one to be reflected; those (if any) which have to be removed are included in the T-contour for C. This implies that it might be possible to see from the T-contour that some of the C-1-inner contours end up inside a region in $\mathcal{M}$. This process might of course have to repeated for some of the D-1-inner contours. When also this process is finished we have arrived at the final set T of contours to be removed.

3. The Estimate

In this section we intend to demonstrate that the construction defined in the preceeding section can lead to a useful bound on the probability of finding the contour C. The probability of finding C is, with w(conf.) for the canonical weight of a configuration, given by

$$p(C) = \sum_{\text{conf.} \ni C} w(\text{conf.}) / \sum_{\text{conf.}} w(\text{conf.}), \tag{3.1}$$

i.e. the canonical weight summed over configurations containing the contour C divided by the total partition function.

As a first step we split the summation over configurations containing C in three parts: The summations over the possible configurations outside C, ext(C), the summation over T-contours containing C as the outer contour, $T \ni C$, and the summation over configurations inside C, which are consistent with T, int(T). This can be done by taking the possible configurations of the interior of C one by one and treating them as described in Section 2; this will then furnish the necessary information for the rearrangement of the summation. One should especially note the refinement introduced in the end of Section 2, which imposes restrictions on the configurations inside C-1-inner contours which are both part of T and inside a region in $\mathcal{M}$.

For fixed T we then keep the following terms in the denominator[2]. The sum over ext(C) is kept unchanged, while in the sum over int(T) for each term in the numerator the corresponding term in the denominator is obtained by first reflecting the configuration inside each region in $\mathcal{M}$

[2] Here we assume that $T^* = T$. The modifications of the argument which would otherwise be necessary should be obvious; Eq. (3.2) will be correct in any case.

in the corresponding reflection line and then deleting T. If this transformation does not cause a term in the denominator to correspond to two or more terms in the numerator, we will be allowed to write

$$p(C) \leqq \sum_{T \ni C} \exp(-\beta\varepsilon L(T)), \tag{3.2}$$

where ε is the lower bound on the energy per unit length of a contour and $L(T)$ is the total length of contours in T.

In order to show the one to one correspondance between terms in the numerator and terms in the denominator, we will show that the process can be reversed. We first note that because in step a in Definition 2.10 we started all over every time T became larger, then the final $\mathscr{M}$ is independent of T in the sense that if T had not been there we would have obtained the same $\mathscr{M}$ from the final set K of C-1-inner contours. We also note that during step b the union of S-contours of all the trees can only grow. If, in Definition 2.8, we now change the order of shapes which are the mirror images of each other and also change the direction of the y-axis then we will obtain the same ordering of the reflected contours as the one we originally had before reflection; except possibly for contours which are ordered by the y-coordinate and not reflected in the same reflection line. However, each of the regions in $\mathscr{M}$ is created independently of the contours in the other regions, so only the ordering inside a region actually matters (here we use that the S-contours grow). Consequently, if we repeat the process of Definition 2.10 with only step b and c, we will obtain the same regions $\mathscr{M}$ from the reflected contours as we did originally.

We can now try to use (3.2) as a basis for estimating a bound on $p(C)$. With an obvious notation we can write (3.2) as:

$$p(C) \leqq \exp(-\beta\varepsilon L(C)) \sum_{T \ni C} \exp[-\beta\varepsilon L(T \backslash C)]. \tag{3.3}$$

According to Definition 2.10 step a, the C-1-inner contours are included into T in units of linear trees. We therefore start by evaluating the contribution from adding one tree. To be precise, we will evaluate a bound on the sum in (3.3) assuming it only involved one linear tree whose S-contour crosses C at a fixed point. As a first step towards simplification, we disregard our knowledge about C (for example we are not using the fact that the C-1-inner contours have to be inside C); we shall also allow crossing to take place between C and any part of the S-contour of the last vertex, although the procedure in step a certainly would allow us to disregard certain parts. This gives a sum over all possible linear trees:

$$\Omega(\beta\varepsilon) = \sum_{\omega} \exp[-\beta\varepsilon L(\omega)], \tag{3.4}$$

where we should remember that the summation includes a summation over possible crossing points.

For practical reasons we shall arrange the sum over ω primarily as a sum over the length of the S-contour of ω. We write, with $s(\omega)$ for the length of the S-contour of ω (the S-contour is necessarily of even length):

$$\Upsilon(k) = \sum_{\substack{\omega \\ s(\omega)=2k}} \exp[-\beta\varepsilon L(\omega)] \tag{3.5}$$

$$\Omega(\beta\varepsilon) = \sum_{k=\sigma}^{\infty} \Upsilon(k), \tag{3.6}$$

where in (3.6) we have introduced σ for the minimal length of a single contour.

We shall write $\Upsilon_1(k)$ for the contribution to $\Upsilon(k)$ from trees which only have one vertex, the root. From a standard argument on the contribution from contours of fixed length one finds

$$\Upsilon_1(k) \leqq \eta \exp[-k(\beta\varepsilon - \zeta)]. \tag{3.7}$$

If the contours are self-avoiding polygons on a lattice with coordination number $q+1$, then one has:

$$\zeta = \log q, \tag{3.8}$$

$$\eta = [(q+1)\, q^{-2}/2k] \cdot 2k = (q+1)\, q^{-2}, \tag{3.9}$$

where the last factor, $2k$, in the expression for η represents the choice of the point of crossing with C.

If $k < 3\sigma$ then $\Upsilon(k) = \Upsilon_1(k)$, but in general a linear tree will of course consist of many vertices. In order to obtain a useful bound on $\Upsilon(k)$ we shall start breaking the tree down in the opposite order to the order in which it was built, i.e. we cut off the last tree added. To describe this we introduce the concept of a generalized linear tree.

Definition 3.1. Let τ be a tree with one branch. The corresponding generalized linear tree, ψ, is then formed from τ by taking the stem in τ and wrapping it up as a single vertex, which is made the root of ψ; the vertices of the branch in τ end up as vertices in ψ with the same connections as in τ; the first vertex in the branch is connected with an edge from the root of ψ. For the root in ψ the S-contour and the R-contour are identical with the S-contour of the corresponding linear tree (the stem of τ) and the reflection number is 0; for the other vertices in ψ the R-contour, the S-contour and the reflection number is as in τ.

If from a normal linear tree ω we cut off the last tree added, what we cut off is a generalized linear tree, ψ, while what remains is a normal linear tree, ω_1. The procedure in Definition 2.10 (more precisely the

choice in step c of which of the two trees is conserved, together with the ordering of the vertices by total s-length in Definition 2.9) ensures that the length of the S-contour of the root in ψ cannot be longer than the S-contour of ω_1.

We now introduce:

$$\theta(1, m, l) = \sum_{\psi} \exp[-\beta\varepsilon L(\psi)], \tag{3.10}$$

where the sum runs over all generalized linear trees with total length of the S-contour equal to $2l$ and with the length of the S-contour of the root at most equal to $2m$. If the sum is empty we put $\theta(1, m, l)$ equal to zero. The reason for introducing the first variable will appear later. We shall include in the summation the choice of two points of connection, one point on the S-contour of the last vertex of ψ and one on the S-contour of the last vertex in the linear tree represented by the root of ψ.

We can now deduce the following inequality:

$$\Upsilon(k) \leqq \Upsilon_1(k) + 2 \sum_{l=\sigma}^{\frac{1}{2}(k-\sigma)} \Upsilon(k-2l)\,\theta(1, k-2l, l). \tag{3.11}$$

The first term comes from the possibility of a linear tree with only one vertex. The bounds on the summation come from the fact that outside the bounds one of the factors is zero. The choice of connection between ω_1 and ψ is correctly represented by the choice of one point on the S-contour of the last vertex in the linear tree which is included in $\Upsilon(k-2l)$, and the choice of one point on the S-contour of the last vertex of the linear tree represented by the root of ψ which is included in $\theta(1, k-2l, l)$. The choice of a connection point on the S-contour of the last vertex in ω is counted as a choice of a point on the S-contour of last vertex in ψ which is included in $\theta(1, k-2l, l)$, and a choice of whether it should be a point on the S-contour of ψ or on the mirror image created by reflection in the reflection line of ω_1 which is included by the Factor 2 in front of the summation. The inequality comes from the disregard of mutual consistency of ω_1 and ψ (i.e. non-overlap of the C-1-inner contours).

If one wants to repeat this process for generalized linear trees one runs into difficulties because the last tree added in a generalized linear tree might have some of its vertices inside the root of the generalized tree. One possibility would then be to break up the root; this would force us to consider trees with more than one branch. Here we shall follow another course which avoids the introduction of new concepts; the idea will be to cut off the last tree added in any tree which now has its root inside the root of the generalized tree. That way we eventually get all the vertices cut off the generalized linear tree, so that we are left with

the root which we already know how to handle since the root represents a linear tree.

To reveal the order of attachment we are going to use the reflection number. When a vertex is created it gets reflection number one; each time it becomes a vertex in a new tree (with a new root) the reflection number is increased by one. When a tree is added to another tree all the vertices which are added are connected in the sense that there is path from the newly created vertex out to all the others. Therefore, if we look at a tree, a vertex with reflection number one represents the addition of a tree, while vertices with higher reflection numbers have been included together with the nearest preceeding vertex with reflection number one. As consequence, in a generalized linear tree we will find the tree we want by looking for the vertex with the lowest reflection number; if this is not unique we take among the possibilities the one furthest out.

To describe what is left of the generalized linear tree after we have cut off a tree which started in a vertex with reflection number p, we introduce $\theta(p, m, l)$. $\theta(p, m, l)$ is defined as $\theta(1, m, l)$ [Eq. (3.10)] except for the following additional restrictions on the terms allowed in the sum over ψ: no vertex (except the root) is allowed to have reflection number lower than p the structure of the root should be consistent with the possibility of attachment of a vertex with reflection number p and the choice of connection point from the last vertex in the generalized linear tree should be consistent with the fact that the vertex which was cut off had reflection number p. For $p=1$ these restrictions are empty, which is consistent with our earlier use of $\theta(1, m, l)$. If the generalized linear tree consists only of the root, then we find

$$\begin{aligned} &\theta_1(p, m, k) = 0\,, \quad && m < k\,, \\ &\theta_1(p, m, k) = 0\,, \quad && k < (2p-1)\,\sigma\,, \\ &\theta_1(p, m, k) \leqq 2^{2-p} k\, \Upsilon(k)\,, \quad && \text{otherwise.} \end{aligned} \tag{3.12}$$

The first equation comes from the requirement that the S-contour of the root should be less than m. The second equation comes from the requirement that one should be able to attach a vertex with reflection number p; the minimal possibility is that the root represents a linear tree with p vertices having reflection numbers $0, 1, 2, \ldots, p-1$, which gives a minimal total S-contour length of $(2^p - 1)\,\sigma$. The occurence of an inequality sign in the last line is caused by the fact that the right hand side is an overestimate if $p > 1$; the first factor represents the forward connection, while the backward connection is included in $\Upsilon(k)$.

By an argument similar to the argument used for the inequality (3.11) we now obtain

$$\begin{aligned}\theta(p,m,k) &\leqq \theta_1(p,m,k)\\ &\quad + \sum_{q=p}^{\pi} 2^{q-p+1} \sum_{j=\sigma}^{\varrho} \theta(q,m,k-2^q j)\,\theta(1,2^{1-q}k-2j,j)\\ \varrho &= 2^{-q}(k+\sigma)-\sigma\\ \pi &= \min\{\log_2(k+\sigma)/2\sigma\,,\quad \log_2(m+\sigma)/\sigma\}\,.\end{aligned} \tag{3.13}$$

The upper bounds are induced by the first two equations in (3.12); the use of $2^{1-q}k-2j$ as the second parameter in the last θ-function is justified as an upper bound on how large the total s-length could have been for the vertex to which the tree represented by this θ-function was attached, [read it $2^{1-q}(k-2^q j)$].

We next intend to use Eqs. (3.7), (3.11), (3.12), and (3.13) to prove the existence of upper bounds:

$$\Upsilon(k) \leqq A\cdot(k+\sigma)^{-n} \tag{3.14}$$

$$\theta(p,m,k) \leqq T(p,m,k) \tag{3.15}$$

$$T(p,m,k) = B\cdot 2^{-2p}(k+\sigma)^{2-n}(m+\sigma)^2\,(m+2k+\sigma)^{-2} \tag{3.16}$$

where A, B, and n are constants depending on σ and the constants occuring in Eq. (3.7). We would carry the proof through recursively if the following inequalities were fulfilled:

$$\eta\exp[-k(\beta\varepsilon-\zeta)] \leqq A(k+\sigma)^{-n}\,,\qquad \sigma\leqq k<3\sigma\,, \tag{3.17}$$

$$\begin{aligned}&\eta\exp[-k(\beta\varepsilon-\zeta)] + 2\sum_{l=\sigma}^{\frac{1}{2}(k-\sigma)} A(k-2l+\sigma)^{-n}\,T(1,k-2l,l)\\ &\qquad\leqq A\cdot(k+\sigma)^{-n}\,,\qquad 3\sigma\leqq k\,,\end{aligned} \tag{3.18}$$

$$\begin{aligned}&T_1(p,m,k)\\ &\quad + \sum_{q=p}^{\pi} 2^{q-p+1} \sum_{j=\sigma}^{\varrho} T(q,m,k-2^q j)\,T(1,2^{1-q}k-2j,j)\\ &\leqq T(p,m,k)\,,\qquad m\geqq\sigma,\,k\geqq\sigma\,,\qquad p\geqq 1\end{aligned} \tag{3.19}$$

$$T_1(p,m,k) = \begin{cases} 0\,, & m<k\\ 0\,, & k<(2^p-1)\,\sigma\\ 2^{2-p}\cdot k\cdot A\cdot(k+\sigma)^{-n}, & \text{otherwise.}\end{cases} \tag{3.20}$$

In the appendix we show that there exist a constant f_0 depending on σ such that if

$$\beta\varepsilon-\zeta\geqq f_0 \tag{3.21}$$

then we can find $A>0$, $B>0$, and choose

$$n=\beta\varepsilon-\zeta \tag{3.22}$$

and have the inequalities (3.17)–(3.19) fulfilled.

Substituting (3.14) into Eq. (3.6) we obtain the following upperbound on the contribution from adding one linear tree, which crosses C at a fixed point.

$$\begin{aligned}\Omega(\beta\varepsilon) &\leqq A\sum_{k=\sigma}^{\infty}(k+\sigma)^{-n} \\ &\leqq A'(2\sigma)^{-n}\end{aligned} \tag{3.23}$$

$$A'=A(1+2\sigma/(n-1))\,. \tag{3.24}$$

Actually we could have any number of linear trees included in T by crossing at given point of C. The total contribution from including linear trees which crosses at a fixed point of C is then bounded by

$$\sum_{j=0}^{\infty}\frac{1}{j!}\,\Omega(\beta\varepsilon)^j\leqq\exp(A'(2\sigma)^{-n})\,, \tag{3.25}$$

i.e. the "free energy" per unit of contour is bounded by

$$f=\varepsilon-\frac{1}{\beta}(\zeta+A'(2\sigma)^{-n}) \tag{3.26}$$

instead of $\varepsilon-\zeta/\beta$. Since linear trees can be included in T not only by crossing with C but with any part of the already existing T, this means that we have to modify the inequalities (3.17) and (3.18) to

$$\begin{aligned}&\eta\exp[-k(\beta\varepsilon-\zeta-A'(2\sigma)^{-n})] \\ &\qquad\leqq A(k+\sigma)^{-n}\,,\quad \sigma\leqq k<3\sigma\,,\end{aligned} \tag{3.17a}$$

$$\begin{aligned}&\eta\exp[-k(\beta\varepsilon-\zeta-A'(2\sigma)^{-n})] \\ &\qquad+2A\sum_{l=\sigma}^{\frac{1}{2}(k-\sigma)}(k-2l+\sigma)^{-n}\,T(1,k-2l,l) \\ &\qquad\leqq A(k+\sigma)^{-n}\,,\quad 3\sigma\leqq k\,.\end{aligned} \tag{3.18a}$$

In the appendix we show that we can determine the bound f_0 such that (3.17a) and (3.18a) together with (3.19) are fulfilled.

As the final result we obtain the following bound on the probability of a given outer contour, C:

$$p(C)\leqq\exp[-L(C)\,(\beta\varepsilon-B(2\sigma)^{-n})]\,, \tag{3.27}$$

$$B=A(1+2\sigma/(f_0-1))\,, \tag{3.28}$$

where n is given by (3.23) and the bound is valid for $n\geqq f_0$. From (3.27) one easily finishes the Peierls' argument in the usual manner.

4. Application to the Hexagonal Lattice and the Diamond Lattice

As a example on the application of the results in the preceeding sections we consider a lattice gas on the hexagonal lattice. We shall consider both the case of nearest neighbour exclusion and nearest neighbour repulsion (equivalent to the antiferromagnetic Ising model).

The hexagonal lattice can be divided into two sublattices, A and B, just as the square lattice such that neighbours in the lattice belongs to opposite sublattices. The A-structure will consist of occupied A-sites and empty B-sites, while the B-structure consists of occupied B-sites and empty A-sites. The contours are drawn between sites with opposite structures. In the case of nearest neighbour repulsion the contours are walks on a triangular lattice and we have $q=5$, $\eta=6/25$, $\zeta=\log 5$, $\sigma=3$. For the nearest neighbour exclusion we can use the additional restriction on the possible structures to reduce q to 3; this gives $\eta=6/9=2/3$, $\zeta=\log 3$, and $\sigma=3$.

If the fugacity per particle is z,

$$\log z=\beta\mu \tag{4.1}$$

then one finds that in the case of nearest neighbour exclusion the loss in number of particles as compared to the close-packed, pure structures is 1/3 per unit of contour. This gives

$$\varepsilon=\mu/3\,. \tag{4.2}$$

For the nearest neighbour repulsion we find that if the repulsion between particles occupying neighbouring sites is a then the bound on the energy per unit length of contour is

$$\varepsilon=\tfrac{1}{2}a-|\mu/3-a/2|\,. \tag{4.3}$$

In view of the complicated transformation used to get from configurations with the contour C to configurations without C, one might worry whether one might get some uncontrolled bulk effect. The easiest way to see that everything works out is to count edges of different types. Inside contours all edges are of the type occupied-unoccupied, while edges crossing contours are either of type occupied-occupied or of type unoccupied-unoccupied. When contours are moved around the crossing edges keep their types, and when contours are removed the edges have their type changed to occupied-unoccupied. Since the number of edges is a constant and the number of particles is uniquely given by the number of edges of the different types, it is clear that the values for ε given in (4.2) and (4.3) are correct and that the method works. Lines which are drawn perpendicular to an edge through the midpoint of the edge are clearly proper reflection lines, i.e. reflection in such a line maps the hexagonal lattice onto itself while the two sublattices are interchanged.

As an example of how to apply the method to a three dimensional lattice we consider the lattice gas with nearest neighbours repulsion on the diamond lattice. Again we can divide the lattice into two sublattices; the A- and B-structures are defined as for the hexagonal lattice. Instead of contours we now make surfaces between sites with different structures and the lines of reflection become planes of reflection. But nothing is changed in principal.

Since the elementary polygons in the diamond lattice are hexagons we have $q=5$, $\zeta=\log 5$, $\eta=6/25$, $\sigma=4$ and we find

$$\varepsilon=\tfrac{1}{2}a-[\mu/4-\tfrac{1}{2}a]\,. \tag{4.4}$$

5. More than Two Structures

Heilmann [8] and Heilmann and Præstgaard [9, 11] have shown how to apply the Peierls' argument to cases with more than two local structures, when each of the structures could be transformed into any of the other structures by translation. It is natural to ask how the method given in Section 2 and 3 of this paper can be extended to cases where one has more than two local structures, each of which can be transformed into any of the other structures by a reflection.

Examples of such models would be second nearest neighbour exclusion on the hexagonal lattice, and third nearest neighbour exclusion on the square lattice (see [11]) and on the triangular lattice. But it is much more important that this class of model includes many models for phase transitions which are connected with the introduction of a preferred direction, e.g. models for liquid crystals, the glass transition, and ferroelectrics.

The problems connected with drawing contours and estimating the free energy per unit of contour were treated in [8] and in great detail in [9], so we shall here limit ourselves to the problems connected with the transformation from a configuration with a contour to a configuration without that contour. In principle one just combines the method of [8] and [9] with the present method.

Because one has more than two structures the contours are no longer simple polygons; they include branch points where three or more lines of contour meat, and the interior of a contour, C, is divide into several regions each having a given structure next to C. The contour, C, is transformed away by treating each of the interior regions separately; the present method of reflection can be used just as well as the original method of translation for this purpose. The only difficulty occurs in connection with C-1-inner contours which have to be deleted. Since we have more than two possible structures, the structure inside a C-1-inner contour do not need to be the same as the structure out-

side C; the problem is solved by the trick already introduced at the end of Section 2 for a similar purpose: treat the interior of a C-1-inner contour which is deleted as the interior of C.

A somewhat more complicated problem arises when the symmetry operation to be used is a rotation of an angle less than 180°; for definiteness we shall consider rotation of 120°. In this case we need two images of contour in order to be able to get a region which is invariant under the rotation; as a consequence we have to change many numbers in the equations in Section 3 (normally the change will be from 2 to 3). To be explicit the following changes occur: in the equations: in (3.5) the condition is changed to $S(\omega) = 3k$. Equation (3.9) is changed to

$$\eta = [(q+1)\, q^{-2}/2k] \cdot 3k = 1.5(q+1)\, q^{-2}\,. \tag{5.1}$$

Equation (3.11) is changed to

$$\Upsilon(k) < \Upsilon_1(k) + 3 \sum_{l=\sigma}^{(k-\sigma)/3} \Upsilon(k-3l)\, \theta(1, k-3l, l)\,. \tag{5.2}$$

In Eq. (3.12) the last two lines read

$$\begin{aligned} &\theta_1(p,m,k) = 0\,, \quad k < \tfrac{1}{2}(3^p - 1)\,\sigma \\ &\theta_1(p,m,k) \leqq 3^{2-p} k\, \Upsilon(k)\,, \quad \text{otherwise.} \end{aligned} \tag{5.3}$$

Equation (3.13) is changed to

$$\begin{aligned} \theta(p,m,k) \leqq \theta_1(p,m,k) + \sum_{q=p}^{\pi} 3^{q-p+1} \sum_{j=\sigma}^{\varrho} \theta(q, m, k-3^q j)\, \theta(1, 3^{1-q}k - 3j, j) \\ \varrho = 3^{-q}(k + \tfrac{1}{2}\sigma) - \tfrac{1}{2}\sigma \\ \pi = \min\{\log_3(2k+\sigma)/3\sigma,\ \log_3(2m+\sigma)/\sigma\}\,. \end{aligned} \tag{5.4}$$

In Eq. (3.16) one should change 2^{-2p} to 3^{-2p} and it might be advantagous to change σ to $\frac{1}{2}\sigma$ and $2k$ to $3k$ (in the last factor). The bounds on k in (3.17) and (3.18) should read $\sigma \leqq k < 4\sigma$ and $4\sigma \leqq k$ respectively. The remaining changes in Eqs. (3.17)–(3.20) are trivial consequence of the earlier changes.

The estimates in the appendix then also have to be changed, but nothing extraordinary happens and once again one concludes that one can choose n as given in (3.22) and find a lower bound on n for the validity of (3.26) and (3.27).

6. Conclusion

From the results given in [6–9, 11] and the results of the present paper it seems possible to conclude that Peierls' argument can be used to prove the existence of a phase transition for a large class of models

with repulsive potential. Let us define the low temperature state as the union of configurations where the energy including one-body contributions (i.e. chemical potential or interaction with magnetic field) is minimal. The effect of unfavorable boundary conditions should not be included or in other words, when an interior configuration has been specified, then the boundary conditions can always be assumed to match the interior configurations. Peierls' argument will then be applicable if the low temperature state possesses the following properties

A. *More than one possible configuration, but only a finite number.*

B. *The possible configurations should be interchangeable by spatial symmetry (or spin reversal).*

Among the still unsettled cases of neighbour exclusion (repulsion) one primarily notes the second nearest neighbour exclusion on the square lattice and the nearest neighbour exclusion on the face centered cubic lattice. In these cases the ground state is infinitely degenerate.

Since the correction to the entropy per unit length of contour introduced by the terms $B\,(2\sigma)^{-n}$ in Eq. (3.27) is bounded and vanishes for $\beta\to\infty$, then it seems fair to expect that one will find similar behavior at low temperature for models fulfilling the above conditions A and B, irrespective of the type of spatial symmetry operation needed to accomplish the interchanged of configurations.

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Appendix

Here we prove that if $\beta\varepsilon-\zeta$ is large enough it is possible to choose values for A, B, and n which fulfills the inequalities (3.17)–(3.19).

We start by finding a bound on the sum in (3.18) assuming that $n\geqq 4.23$. We have

$$\tfrac{1}{2}(k+\sigma)^{n-2}\sum_{l=\sigma}^{\frac{1}{2}(k-\sigma)}[(k+\sigma-2l)(l+\sigma)]^{2-n}=c_1+c_2\,, \tag{A.1}$$

$$\begin{aligned} c_1&=\tfrac{1}{2}(k+\sigma)^{n-2}\sum_{l>\frac{1}{2}(k-3\sigma)}^{\frac{1}{2}(k-\sigma)}[(k+\sigma-2l)(l+\sigma)^{2-n}\\ &\leqq\tfrac{1}{2}\sigma^{3-n}\,, \end{aligned} \tag{A.2}$$

$$\begin{aligned} c_2&=\tfrac{1}{2}(k+\sigma)^{n-2}\sum_{l=\sigma}^{\frac{1}{2}(k-3\sigma)}[(k+\sigma-2l)(l+\sigma)]^{2-n}\\ &\leqq(k+\sigma)^{n-2}\sum_{l=\sigma}^{(k-\sigma)/4}[(k+\sigma-2l)(l+\sigma)]^{2-n}\,. \end{aligned} \tag{A.3}$$

For $k<5\sigma$ one has $c_2=0$; for $k=5\sigma$:

$$c_2=\tfrac{1}{2}\cdot(3/4\sigma)^{n-2} \tag{A.4}$$

for $5\sigma<k\leqq 9\sigma$ one has

$$\begin{aligned} c_2 &\leqq \left(1+\frac{1}{4}(k-5\sigma)\right)(k+\sigma)^{n-2}\,[(k-\sigma)\,(2\sigma)]^{2-n} \\ &\leqq (1+\sigma)\,(3/4\sigma)^{n-2}\,. \end{aligned} \tag{A.5}$$

For $k>9\sigma$ we write

$$\begin{aligned} c_2 &\leqq c_3+c_4 \\ c_3 &= (k+\sigma)^{n-2}\sum_{l=\sigma}^{(k-\sigma)/8}[(k+\sigma-2l)\,(l+\sigma)]^{2-n} \\ &\leqq (k+\sigma)^{n-2}\,[(k-\sigma)\,2\sigma]^{2-n} \\ &\quad +(k+\sigma)^{n-2}\int_{\sigma}^{(k-\sigma)/8} dl[(k+\sigma-2l)\,(l+\sigma)]^{2-n} \\ &\leqq \left[\frac{k+\sigma}{(k-\sigma)\,2\sigma}\right]^{n-2}+\frac{4\sigma}{(n-3)}\left[\frac{(k+\sigma)}{(k-\sigma)\cdot 2\sigma}\right]^{n-2} \end{aligned} \tag{A.6}$$

$$\leqq [1+4\sigma/(n-3)]\,(5/8\sigma)^{n-2} \tag{A.7}$$

$$\begin{aligned} c_4 &= (k+\sigma)^{n-2}\sum_{l>(k-\sigma)/8}^{(k-\sigma)/4}[(k+\sigma-2l)\,(l+\sigma)]^{2-n} \\ &\leqq \frac{1}{8}(k-\sigma)\left[\frac{(k+\sigma)\cdot 32}{(3k+5\sigma)\,(k+7\sigma)}\right]^{n-2} \\ &\leqq \sigma(5/8\sigma)^{n-2}\,. \end{aligned} \tag{A.8}$$

(Here we use $n\geqq 4.23$). Collecting (A.4–8) we find

$$c_2\leqq(3/4\sigma)^{n-2}\,(1+\sigma+4\sigma/(n-3))\,. \tag{A.9}$$

and the inequality (3.18) will consequently be implied by

$$(\eta/A)\exp[-k(\beta\varepsilon-\zeta)]\,(k+\sigma)^n+B\cdot a_1(\sigma,n)\leqq 1 \tag{A.10}$$

$$a_1(\sigma,n)=\tfrac{1}{2}\sigma^{3-n}+[1+\sigma+4\sigma/(n-3)]\,(3/4\sigma)^{n-2}\,. \tag{A.11}$$

We next turn to (3.19); the sum of interest in this case is:

$$\begin{aligned} c_5 &= 2^p(k+\sigma)^{n-2}\sum_{q=p}^{\pi}2^{-q-1}\sum_{j=\sigma}^{\varrho}[(k+\sigma-2^q j)\,(j+\sigma)]^{2-n} \\ &\quad\cdot\left[\frac{(2^{1-q}k-2j+\sigma)\,(m+2k+\sigma)}{(2^{1-q}k+\sigma)\,(m+2k+\sigma-2\,2^q j)}\right]^2 \end{aligned} \tag{A.12}$$

where ϱ and π are given by (3.13). Since $\pi\geqq q$ implies

$$2^q\sigma\leqq m+\sigma\,, \tag{A.13}$$

one concludes

$$\frac{(2^{1-q}k-2j+\sigma)(m+2k+\sigma)}{(2^{1-q}k+\sigma)(m+2k+\sigma-2\cdot 2^q j)} \leqq 1 \tag{A.14}$$

which means that

$$\begin{aligned} c_5 &\leqq 2^p(k+\sigma)^{n-2}\sum_{q=p}^{\pi}2^{-q-1}\sum_{j=\sigma}^{\varrho}[(k+\sigma-2^q j)(j+\sigma)]^{2-n} \\ &\leqq c_6+c_7+c_8 \end{aligned} \tag{A.15}$$

$$c_6 = 2^p(k+\sigma)^{n-2}\sum_{q=p}^{s}2^{-q-1}\sum_{j=\sigma}^{r}[(k+\sigma-2^q j)(j+\sigma)]^{2-n} \tag{A.16}$$

$$c_7 = 2^p(k+\sigma)^{n-2}\sum_{q>s}^{t}2^{-q-1}\sum_{j=\sigma}^{\varrho}[(k+\sigma-2^q j)(j+\sigma)]^{2-n} \tag{A.17}$$

$$c_8 = 2^p(k+\sigma)^{n-2}\sum_{q=p}^{s}2^{-q-1}\sum_{j>r}^{\varrho}[(k+\sigma-2^q j)(j+\sigma)]^{2-n} \tag{A.18}$$

$$s = \log_2[(k+\sigma)/3\sigma]\,, \tag{A.19}$$

$$t = \log_2[(k+\sigma)/2\sigma]\,, \tag{A.20}$$

$$r = \varrho-\sigma = 2^{-q}(k+\sigma)-2\sigma\,. \tag{A.21}$$

$$\begin{aligned} c_6 &\leqq (k+\sigma)^{n-2}\sum_{q=p}^{s}2^{p-q}\sum_{j=\sigma}^{\frac{1}{2}}[(k+\sigma-2^q j)(j+\sigma)]^{2-n} \\ &= c_9+c_{10}+c_{11}\,. \end{aligned} \tag{A.22}$$

$$c_9 = (k+\sigma)^{n-2}\sum_{q=p}^{u}2^{p-q}\sum_{j=\sigma}^{\varrho/4}[(k+\sigma-2^q j)(j+\sigma)]^{2-n} \tag{A.23}$$

$$u = \log_2[(k+\sigma)/5\sigma]\,. \tag{A.24}$$

$$\begin{aligned} &\sum_{j=\sigma}^{\varrho/4}[(k+\sigma-2^q j)(j+\sigma)]^{2-n} \\ &\leqq [(k+\sigma-2^q\sigma)(2\sigma)]^{2-n}+\int_{\sigma}^{\varrho/4}dj(k+\sigma-2^q j)(j+\sigma)^{2-n} \\ &\leqq [(k+\sigma-2^q\sigma)(2\sigma)]^{2-n}(1+4\sigma/(n-3))\,. \end{aligned} \tag{A.25}$$

$$\begin{aligned} c_9 &\leqq (k+\sigma)^{n-2}(1+4\sigma/(n-3))\sum_{q=p}^{u}2^{p-q}[(k+\sigma-2^q\sigma)(2\sigma)]^{2-n} \\ &\leqq 2(1+4\sigma/(n-3))\left[\frac{k+\sigma}{(4(k+\sigma)/5)(2\sigma)}\right]^{n-2} \\ &\leqq 2(1+4\sigma/(n-3))(5/8\sigma)^{n-2}\,. \end{aligned} \tag{A.26}$$

$$\begin{aligned} c_{10} &= (k+\sigma)^{n-2}\sum_{q=p}^{u}2^{p-q}\sum_{j>\varrho/4}^{\frac{1}{2}\varrho}[(k+\sigma-2^q j)(j+\sigma)]^{2-n} \\ &= (k+\sigma)^{n-2}\sum_{j>\sigma}^{\frac{1}{2}\varrho}(j+\sigma)^{2-n}\sum_{q\geqq v}^{w}2^{p-q}(k-2^q j+\sigma)^{2-n}, \end{aligned} \tag{A.27}$$

$$\varrho = 2^{-p}(k+\sigma) - \sigma\,, \tag{A.28}$$

$$v = \max\{p, \log_2[(k+\sigma)/(4j+\sigma)]\}\,, \tag{A.29}$$

$$w = \log_2[(k+\sigma)/(2j+\sigma)]\,. \tag{A.30}$$

$$\begin{aligned} c_{10} &\leqq \sum_{j>\sigma}^{\frac{1}{2}\varrho} \left[\frac{2j+\sigma}{(j+\sigma)^2}\right]^{n-2} \\ &\leqq \int_{\sigma}^{\infty} dj \left[\frac{2j+\sigma}{(j+\sigma)^2}\right]^{n-2} \\ &\leqq \frac{9}{4(n-3)}\left(\frac{3}{4\sigma}\right)^{n-3} \end{aligned} \tag{A.31}$$

$$\begin{aligned} c_{11} &= (k+\sigma)^{n-2} \sum_{q>u}^{s} 2^{p-q} \sum_{j=\sigma}^{\frac{1}{2}\varrho} [(k+\sigma-2^q j)(j+\sigma)]^{2-n} \\ &\leqq (k+\sigma)^{n-2} \cdot \sigma[(2\sigma)(\tfrac{3}{5}(k+\sigma))]^{2-n} = \sigma(5/8\sigma)^{n-2}\,. \end{aligned} \tag{A.32}$$

$$\begin{aligned} c_7 &\leqq (k+\sigma)^{n-2} \cdot \tfrac{1}{2}\sigma \max_q \{[(2^{-q}(k+\sigma))(2^q\sigma)]^{2-n}\} \\ &= \tfrac{1}{2}\sigma^{3-n}\,. \end{aligned} \tag{A.33}$$

$$c_8 \leqq \sigma^{3-n}\,. \tag{A.34}$$

Collecting (A.15), (A.22), (A.26), (A.31), (A.32), (A.33) and (A.34), we obtain

$$c_5 \leqq a_2(\sigma, n)\,, \tag{A.35}$$

$$\begin{aligned} a_2(\sigma, n) &= (5/8\sigma)^{n-2}(2 + 8\sigma/(n-3)) \\ &\quad + (3/4\sigma)^{n-3}\, 2.25/(n-3) \\ &\quad + \sigma(5/6\sigma)^{n-2} + (3/2)\,\sigma^{3-n}\,. \end{aligned} \tag{A.36}$$

In order to transform the inequality (3.19) into a suitable form we also need for $m \geqq k \geqq (2^p - 1)\,\sigma$:

$$\begin{aligned} &2^{2-p} \cdot k(k+\sigma)^{-n} \cdot 2^{2p}(k+\sigma)^{n-2}(m+\sigma)^{-2}(m+2k+\sigma)^2 \\ &\quad = 2^{p+2} k \left[\frac{m+2k+\sigma}{(m+\sigma)(k+\sigma)}\right]^2 \\ &\quad \leqq 4k(3+\sigma)^2\,(k+\sigma)^{-3} \leqq 8\,. \end{aligned} \tag{A.37}$$

The inequality (3.19) will therefore be implied by:

$$8A/B + Ba_2(\sigma, n) \leqq 1\,. \tag{A.38}$$

For $n \geqq 4$, $\sigma \geqq 1$ one finds that

$$a_2(\sigma, n) \leqq 7.75 \tag{A.39}$$

which means that (A.38) is certainly fulfilled for

$$A = 1/256\,, \qquad B = 1/16\,. \tag{A.40}$$

Since for $n \geqq 4$, $\sigma \geqq 1$ we also have

$$a_1(\sigma, n) \leqq 4 \tag{A.41}$$

then (A.10) would be satisfied if

$$256\eta \exp[-k(\beta\varepsilon - \zeta) + n \log(k+\sigma)] \leqq 3/4 . \tag{A.42}$$

Just (3.18) is implied by (A.42), (3.19) is implied by

$$256\eta \exp[-k(\beta\varepsilon - \zeta) + n \log(k+\sigma)] \leqq 1 . \tag{A.43}$$

We want (A.42) satisfied for $k \geqq 3\sigma$ and (A.43) satisfied for $\sigma \leqq k < 3\sigma$; with the choice for n given in (3.22):

$$n = \beta\varepsilon - \zeta \tag{A.44}$$

we find that the determining inequality is

$$256\eta \exp[-n(\sigma - \log 2\sigma)] \leqq 1 \tag{A.45}$$

which for $\sigma \geqq 1$ always can be satisfied for n large enough.

We actually want (3.17a) and (3.18a) satisfied; therefore (A.45) should be altered to

$$256\eta \exp[-n(\sigma - \log 2\sigma - \tfrac{1}{256}(1 + 2\sigma/(n-1))(2\sigma)^{-n})] \leqq 1 . \tag{A.46}$$

However, this inequality can also be satisfied if n is large enough which proves the assertion after (3.18a).

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O. J. Heilmann
Department of Chemistry
H. C. Ørsted Institute
DK-2100 Copenhagen, Denmark