enumeration (not necessarily as the same segment). Thus, it is wasteful to
generate such walks repeatedly; our technique has been to generate walks
of moderate length beforehand, and to keep their details readily available
in a major area of computer memory.

This in itself would already make the program very fast in execution. A
further substantial increase in speed (of a factor of 2 or 3) is obtained by
noticing that it is now never necessary to lay the ordinary sites of the final
segment on the lattice (and, by implication, to remove them later); such
sites are already mutually self-avoiding as a result of their generation at the
preliminary stage. All that is needed for the final segment is to check that the
ordinary sites can be laid on the lattice without interfering with the earlier
segments of the configuration. Provided that the program information is
properly organised, such a test is very simple to carry out. In our version of
the program the test is coded as a loop of only seventeen computer instruc-
tions for the IBM360. This program fragment has been designed with great
care, as it is estimated that in some enumerations (in particular on the f.c.c.
lattice) it may be executed for 90% or 95% of the total running time.

A condensed flowchart for the process is shown in Fig. 8, the upper part
of which shows how the topology vertices are staked out, while the lower
part describes the procedure for filling in the bridges. Each part has the basic
structure of Fig. 3, though it should be noted that the parameters \( j_1 \) and \( j_2 \)
here label segments and not points. Where the words select and find appear
in heavy type, they refer to the body of information about self-avoiding walks
which is assumed to be already available in the store.

Programs embodying these principles have been written for the National
Physical Laboratory ACE (now obsolete), the English Electric KDF9 and
the IBM360 computers. In favourable cases, topology embeddings have
been counted at speeds of about 10^6 successes per minute (on the IBM360).

References

There is much published work in statistical physics which relies heavily on
configuration-counting by computer. Not many publications give details of
computing procedures, however, and it seems inappropriate to list them here; in
any case, they are almost certainly to be found in the bibliographies of the other
articles in this volume. An exception is W. F. Lunnon, (1971), “Counting Poly-
ominos” : article in “Computers in Number Theory” (A. O. L. Atkin and B. J.

3. Linked Cluster Expansion

Michael Wortis*

Department of Physics, University of Illinois at
Urbana-Champaign, Urbana, Illinois, U.S.A.

I. Introduction .................................................. 114
A. Motivation .................................................. 114
B. Derivation of series expansion ............................... 116
C. The linked-cluster expansion: historical .................. 117
D. Format and aim of this article .............................. 119

II. The Linked-cluster Expansion with Commuting Variables: The Ising Model 120
A. Notation and preliminaries .................................. 120
B. Unrenormalised linked-cluster expansion .................. 122
  Graphical definitions I ...................................... 124
  Rule 1: free energy \( W \), unrenormalised form .............. 125
  Rule 2: renormalised semi-invariants, unrenormalised form ..... 129
  Rule 3: pair correlations, unrenormalised form .............. 130
C. Proof of the unrenormalised linked-cluster expansion .......... 131
D. Relation of the linked-cluster and weak-embedding expansions for
   the free energy .............................................. 133
E. Vertex renormalisation: the correlations ................... 135
  Graphical definitions II .................................... 137
  Rule 4: self-field, unrenormalised form ..................... 138
  Rule 5: pair correlations, vertex renormalised form .......... 140
  Rule 6: self-field, vertex renormalised form ................. 140
F. Vertex renormalisation: the free energy................... 141
  Rule 7: the functional \( \Phi \), vertex renormalised form .......... 142
G. The classical-fluid linked-cluster expansion as a special case 144
  Rule 8A: classical-fluid free energy \( W \), unrenormalised \( \Phi \)-form ........ 146
  Rule 8B: classical-fluid free energy \( W \), unrenormalised \( f \)-form ...... 147
  Rule 9: classical-fluid self-field, vertex renormalised \( f \)-form ....... 147
  Rule 10: classical-fluid functional \( \Phi \), vertex renormalised \( f \)-form. 148
H. \( \Phi \)-derivable approximations ............................. 148

* This work was supported by National Science Foundation Grant Number NSFP16886
I. Introduction

A. Motivation

The study by the method of perturbative series expansions of the thermodynamic properties of models described by lattice Hamiltonians has historically been of great value in the understanding of critical phenomena. Onsager’s brilliant solution of the two-dimensional nearest-neighbour zero-field spin $\frac{1}{2}$ Ising model (Onsager, 1944) proved beyond question that mean-field, Landau-like descriptions of the critical region were qualitatively, quantitatively, and fundamentally false. On the other hand, Onsager’s methods and those used by subsequent workers in obtaining rigorous solutions for particular one- and two-dimensional models were quite specialised and have done little to suggest viable techniques for first-principle calculations—even approximate—of the critical properties of more complicated systems, particularly in three dimensions. Ideally a general technique is required, embodying a physically correct understanding of the large fluctuations dominating the singular, critical behaviour and from which all relevant quantities could be calculated qualitatively accurately and to any desired degree of precision, given only the requisite labour. Such a general technique is not currently available, though recent Russian work (Gribov and Migdal, 1969; Migdal, 1969, 1970; Polyakov, 1969, 1970) may point in the right direction. Series expansions, although they provide little physical understanding of the critical processes, have made possible precise and reliable estimates of a variety of critical properties for a wide class of model systems. Critical exponents derived from series were important data in the formation of the scaling hypothesis (Essam and Fisher, 1963; Fisher, 1965; Kadanoff, 1966; Kadanoff et al., 1967; Widom, 1965a, b; Domb and Hunter, 1965). Similarly, series-derived model information is often compared quantitatively with measurements in the analysis of experimental data. This chapter will attempt neither a review of important results derived by series methods nor a detailed assessment of the contribution of these results to the understanding of critical phenomena. The interested reader is referred to several useful review articles (Domb, 1960; Fisher, 1963, 1965, 1967; Helfand, 1963). Our present focus is methodology rather than results.

Domb and Sykes (Domb, 1949, 1960; Domb and Sykes, 1956, 1957, 1961) were the first to develop series methods for the study of critical phenomena. The volume of subsequent work, following this initial exploration, has been considerable. Many refinements of techniques and extensions to other model systems are discussed elsewhere in this volume; however, the main lines of the original work remain clear. There are three stages in the argument:

(i) a parameter $x$ is selected in terms of which the desired thermodynamic or correlation function of the chosen model system may perturbatively be expanded;

(ii) a finite number of coefficients in the perturbation series expansion are computed;

(iii) extrapolative analysis of the computed coefficients in the light of the expected form of the critical behaviour locates the critical point and gives estimates of singular behaviour.

The parameter $x$ selected at stage (i) is often a typical interaction energy (such as the exchange energy $J$) divided by the thermal energy $kT = \beta^{-1}$, $x = \beta J$. For certain special cases such as the Ising model the low-temperature parameter $x = \exp(-\beta J)$ may also be used. The quantity $Q$ whose critical behaviour as a function of $x$ is to be studied must have an expansion about $x = 0$,

$$Q(x) = \sum_{n=0}^{\infty} a_n x^n,$$

with a finite radius of convergence. At stage (ii) a finite number of the coefficients $a_n$ are determined, $a_0, a_1, \ldots, a_{n_{\text{max}}}$. Typically the calculation is in principle straightforward; however, the increased labour necessary for calculating each succeeding coefficient is large. A rule of thumb is that the
computation of $a_{n+1}$ involves at least as much labour as the cumulative calculation of $a_0, \ldots, a_n$. Thus, while there is in principle no limit to the number of calculable coefficients, there is in practice a rather sharp upper bound $n_{\text{max}}$ (which depends on the details of the model being considered) determined by such practical considerations as time and patience and, at the next level, electronic computer capacity and funding. Finally at stage (iii) critical properties are extracted from the available coefficients by methods described in this volume (Gaunt and Guttmann, Chapter 4) and elsewhere (Baker, 1965; Domb and Sykes, 1961; Fisher, 1967).

The limiting link in the above schema is stage (ii), determination of the expansion coefficients. Typically the first few coefficients are trivial and no special methodology is necessary. However, in higher orders the bookkeeping is extremely involved; and, scrupulous accuracy is necessary in determining the coefficients, since (in stage (iii)) extrapolation makes apparent critical-point behaviour exceedingly sensitive to tiny fractional changes in the last few available coefficients. For these reasons, it becomes of paramount importance to have a well-defined, systematic procedure for computing coefficients, which incorporates as many short cuts as possible and minimises the opportunity for careless error. It is to this systematisation which we now turn.

B. Derivation of series expansions

All systematic methods for the determination of series coefficients are at some level graphical or diagrammatic. With each coefficient is associated a set of graphs of some given topological type. To each graph corresponds a numerical contribution according to a well-defined rule. To calculate the required coefficient, one simply sums all contributions. There are, thus, three steps in the calculation:

(i) enumerate the contributing graphs;
(ii) calculate the contribution of each;
(iii) add.

Accordingly, graphical methods differ in (a) which diagrams contribute and (b) what rules determine the contributions.

The rule for calculating the contribution (ii) of each graph generally consists of two parts:

(a) a factor, the weight of the graph, which depends only on its topology, and
(b) the configurational multiplicity of the graph, determined by the number of different ways it can be embedded in the underlying lattice subject to certain constraints.

Different graphical expansions differ with respect to both weights and embedding constraints. The three main embedding systems are strong, weak, and free (Domb, 1960; Sykes et al., 1966; Jasnow, 1969; Jasnow and Wortis, 1968) in order of decreasingly stringent constraints. The strong and weak systems are discussed elsewhere in this volume (Chapter 1), and the relation between them has been investigated by Sykes et al. (1966). The free embedding system and its relation to the weak system is considered in the appendix to this article.

In high-order calculations the number of graphs which potentially contribute in (i) above is enormous. Many of these may have no possible embeddings once the constraints (b) have been applied. Broadly speaking, the more restrictive the constraints, the fewer the possible embeddings. This very significant simplification favours restrictive expansions.

An alternative and in many ways complementary method of cutting down the number of contributing graphs is to perform a selective resummation or renormalisation in which classes of graphs with related topologies are lumped together. The calculation of the weights (a) of the remaining graphs is then more complicated, and the net effect is a trade-off of algebraic complexity for topological complexity. The special simplicity of the configurational factors (b) for the free or unrestricted embeddings makes the renormalisation method most appropriate. As a rule the restrictive embeddings are best in low dimensionality and for rather open lattice structures. For close-packed lattices and in higher dimensionality the renormalisation method seems preferable. In any given study, there may be additional considerations favouring one method or another. For example, for the high-temperature Ising model the weak-embedding method (Section II.D) becomes increasingly complex for higher spin, while for the free-embedding linked-cluster expansion the spin enters merely as a parameter.

This article will deal exclusively with the free-embedding expansions and their renormalisation. Connection with the weak-embedding expansion is discussed in Section II.D for the $s = \frac{1}{2}$ Ising model.

C. The linked-cluster expansion: historical

The prototypical free-embedding expansion is the linked-cluster expansion for the classical fluid, dating from the work of Ursell (1927), Yvon (1935), and Mayer (1937). Good reviews of more recent work are given by Uhlenbeck and Ford (1962) and by Stell (1964) (see also Chapter 1). The original expansion is in terms of the non-interacting single particle density $n_0$, with the pair-potential in the combination $[\exp (-\beta\epsilon(r_1 - r_2)) - 1]$ as expansion.

† We shall use the terminology "graph" rather than "linear graph" or "diagram." Although an extensive mathematical literature on graph theory exists (Berge, 1958; Harary, 1969; Ore, 1962), physicists have been far from universal in adopting its terminology. We shall introduce terminology in detail as we proceed, conforming in general to the recent compilation of Essam and Fisher (1970). (See also Domb, this volume, Chapter 1).
The generalisation of the Englert formalism to the spin $s$ quantum mechanical Heisenberg model was first done by Stinchcombe et al. (1963). It was not until the work of Yaks et al. (1968a, b), who employed a partial one-particle renormalisation, that the expansion was used systematically in calculations. The full renormalisations are carried out in Section III.D, where strong parallels with the quantum fluid are pointed out. However, in the calculation of those high-temperature series of relevance to the study of critical phenomena, no form of the linked-cluster expansion has yet been made competitive with the weak-embedding method of Baker et al. (1967) for the $s = 1/2$ Heisenberg model (see also this Volume, Chapter 5).

In studying the properties of an assembly of electrons on a lattice, interacting via a zero-range interaction, Hubbard (1963, 1964a, b, 1965, 1966) has developed a linked-cluster expansion in powers of the kinetic energy, structurally identical to the unrenormalised expansion for the quantum Heisenberg model, only with the added complication of Fermi statistics.

### D. Format and aim of this article

The intent of this article is frankly pedagogical. We hope to make the linked-cluster expansion for systems like the Ising and Heisenberg models available to the reader as a working tool. To this end we have included a considerable number of simple, worked examples. While these may strike the initiate as superfluous, it is hoped that the non-expert may find them useful. The central results of the theory are the rules (in the sense of I.B (i)-(iii)) for writing down the original graphical expansions and their renormalisations. From a practical point of view, the important thing is to be able to apply the rules in actual calculation. Characteristically, the detailed derivation of the rules, while logically necessary, is often not very illuminating. Such derivations tend to involve cumbersome combinatorial arguments with little obvious physical meaning. Without pretending to rigor, we have attempted to sketch all important steps and to point out—often by a simple example—what the essential topological content of the general proof must be. References are given to more detailed proofs, when they are available in the literature.

The usefulness of the linked-cluster expansion is by no means restricted to the derivation of series expansions for critical properties. Many approximate closed-form solutions for thermodynamic and correlation functions can be derived by graphical methods by selective truncation of graphical sums. Despite much effort, no such approach has yet yielded correct properties in the critical region; however, qualitatively correct phase diagrams and quantitative non-critical results can be obtained for a variety of systems. While our primary orientation is towards the derivation of series expansions for problems in critical phenomena, we have attempted to develop the theory in
such a way that it applies immediately to a variety of non-critical calculations as well.

The methods illustrated are sufficiently general to apply to any system which is spatially local in the absence of the perturbing interaction. For the sake of clarity it seemed wise, however, to couch the discussion in terms of specific examples. Directions of possible generalisation are remarked.

Section II develops the linked-cluster expansion and its various renormalisations for the spin $s$ Ising model. This development, which illustrates all the topological content of the renormalisation method in the simplest possible context, is carried through in full detail. Section II.D explores the relation between the linked-cluster and weak-embedding expansions for the $s = \frac{1}{2}$ Ising model. Section II.G shows how the magnetic expansion reduces for the classical fluid to the Ursell–Yvon–Mayer expansion.

In Section III linked-cluster expansions for a variety of other more complicated systems are sketched. The topological content of these expansions and their renormalisations are identical to those of the Ising model. Omitting redundant derivations, we have attempted to bring out the parallels with the Ising development. Once these are understood, all results may be written down by inspection.

II. The Linked-Cluster Expansion with Commuting Variables: The Ising Model

A. Notation and preliminaries

The Hamiltonian for the spin $s$ Ising model is usually written,

$$\mathcal{H} = -\frac{1}{s} \sum_{\langle ij \rangle} J_{ij} s_i s_j - \frac{m}{s} \sum_i H_i s_i,$$

where $\sum_{\langle ij \rangle}$ denotes the sum over distinct pairs. Each spin $s_i (i = R_1, \ldots, R_N)$ is situated at one of the $N$ sites of a regular lattice and interacts via its $z$-component magnetic moment $m s_i \mathbf{s}$ ($s_i = -s, -s + 1, \ldots, s$) with an inhomogeneous external magnetic field $(1/s)H_i$. Each spin pair is coupled by the spin-dependent energy $(-J_{ij}/s^2)s_is_j$, where the exchange coupling $J_{ij}$, which may in principle be different for each pair, is normally a function only of the difference variable $(R_i - R_j)$. Note that $J_{ii} = 0$. The factors of $1/s$ are chosen so as to normalise the maximum interaction between parallel spins. The classical limit, in which the spins become classical unit vectors, is achieved by taking $s \to \infty$.

It will be convenient to introduce as variables the operators $\mu = s_i/s$, which range in the interval $[-1, 1]$. We then rewrite (1) in terms of dimensionless variables,

$$-\beta \mathcal{H} = \frac{1}{s} \sum_{\langle 12 \rangle} p(12) \langle \mu(1) \mu(2) \rangle + \sum_i h(1) \mu(1),$$

where $\beta = 1/kT$ and the numerical arguments, which will henceforth stand for lattice sites, run over the points $R_1, \ldots, R_N$. The dimensionless exchange coupling is $\epsilon(ij) = \beta J_{ij}$; the reduced magnetic field is $h(i) = \beta m H_i$. The partition function and free energy of the Ising model are given by

$$\text{Tr} \exp (-\beta \mathcal{H}) = Z[h, v] = \exp W[h, v]$$

and

$$F = -kT W[h, v],$$

where the functional dependence of the thermodynamics on the fields and exchange couplings has been emphasised by the use of square brackets.

The advantage of maintaining the fields and couplings variable independently for each site and pair is that all correlation functions may be found by differentiation directly from the dimensionless free energy $W$. For example,

$$\mathcal{M}_1(1) \equiv \langle \mu(1) \rangle = \frac{1}{Z} \frac{\delta Z}{\delta (\beta h(1))} = \frac{1}{Z} \frac{\delta W}{\delta h(1)} = \frac{dW}{d(\beta m H_1)}. \quad (4)$$

We use the standard notation $\langle X \rangle = (1/Z) \text{Tr} X \exp (-\beta \mathcal{H})$. By using the functional notation for the derivative $\delta W/\delta h$, we stress that it is the local field at the site 1 which is being varied. Similarly, the two-point (cumulant) correlations are available as second derivatives:

$$\mathcal{M}_2(12) \equiv \langle \mu(1) \mu(2) \rangle - \langle \mu(1) \rangle \langle \mu(2) \rangle = \frac{\delta^2 W}{\delta h(1) \delta h(2)} = \langle \mu(1) \mu(2) \rangle. \quad (5)$$

The $n$-point (cumulant) correlations are defined by

$$\mathcal{M}_n(1 \ldots n) \equiv \frac{\delta^n W}{\delta h(1) \ldots \delta h(n)} = \frac{\delta W}{\delta h(n)}, \quad n = 1, 2, \ldots. \quad (6)$$

Derivatives of $W$ with respect to the pairwise exchange couplings also generate correlations:

$$\frac{\delta W}{\delta \epsilon(12)} = \langle \mu(1) \mu(2) \rangle, \quad (7)$$

which can be rewritten using (4) and (5) in the general form,

$$\frac{\delta W}{\delta \epsilon(12)} = \frac{\delta^2 W}{\delta h(1) \delta h(2)} = \frac{\delta W}{\delta h(1) \delta h(2)} + \frac{\delta W}{\delta h(1) \delta h(2)}. \quad (8)$$
Equation (8) constitutes a non-linear functional differential equation for the free energy. The appropriate initial condition is

\[ W[h, v = 0] = W_0[h] = \ln \text{Tr} \exp \left( \sum_1 \mu(1) \right) = \sum_1 M_0(1), \quad (9) \]

with

\[ M_0[1; h(1)] = \ln \left[ \sum_{n=1}^1 e^{\mu(1)n} \right] = \ln \frac{\sinh \left( \frac{h(1)}{2} (2s + 1) \right)}{\sinh \left( \frac{h(1)}{2s} \right)}, \quad (10) \]

which is even in \( h \). While the system (8)–(10) cannot in general be solved, it can be used to develop \( W \) in powers of \( v \). This development, interpreted graphically, is just the linked-cluster expansion for the Ising model free energy \( W \). Once \( W \) is known, eqn (6) yields the corresponding linked-cluster expansions for all correlation functions. In actual calculation—i.e. once the graphical rules are known—it is often most convenient (Stanley and Kaplan, 1966; Stanley, 1967) to find the correlations directly and evaluate physical quantities from them. For example, the susceptibility per site and the total energy are respectively (in dimensionless variables),

\[ \chi = \sum_{1,\alpha} \mathcal{M}_2(12), \]

\[ -E = \frac{1}{2} \sum_{1,2} v(12) \left[ -\mathcal{M}_2(12) + \mathcal{M}_1(1) \mathcal{M}_1(2) \right] + \sum_1 h(1) \mathcal{M}_1(1). \]

B. Unrenormalised linked-Cluster expansion

The linked-cluster expansion for \( W[h, v] \) is nothing more than the many-variable Taylor development,

\[ W[h, v] = \left[ \exp \left( \sum_{\text{pairs}} v(12) \frac{\delta}{\delta \bar{v}(12)} \right) \right] W[h, \bar{v}] \bigg|_{\bar{v} = 0}. \quad (11) \]

The first few terms read,

\[ W[h, v] = W_0[h] + \sum_{1,2} v(12) \frac{\delta}{\delta \bar{v}(12)} W[h, \bar{v}] \bigg|_{\bar{v} = 0} + \frac{1}{2} \sum_{1,2,3,4} v(12)v(34) \frac{\delta}{\delta \bar{v}(34)} \left[ W[h, \bar{v}] \bigg|_{\bar{v} = 0} + \ldots \right. (12) \]

In each order the coefficient of \( v^n \) has the form of \( \frac{\delta^n W}{\delta v^n} \bigg|_{v=0} \), which by successive use of (8) can always be expressed in terms of products of the correlation functions \( \mathcal{M} \) evaluated in the non-interacting limit \( v = 0 \). At \( v = 0 \), all the lattice sites are entirely uncorrelated with one another, so the correlations are spatially local,

\[ \mathcal{M}_n(1 \ldots n)|_{v=0} = \delta(1 \ldots n) M_n(1), \quad (13) \]

where \( \delta(1 \ldots n) = 1 \) when all lattice points, 1, \ldots, \( n \), are identical and vanishes otherwise. The quantities \( M_n(1) \) are called bare or unrenormalised semi-invariants (Englert, 1963). Note that \( M_n(1) \) depends only on the field \( h(1) \) at the site 1. It follows from (9) and (6) that

\[ \frac{d^n}{dh^n} M_n(h), \quad (14) \]

or

\[ W_0[h] = \sum_{1,2} \sum_{n=0}^\infty \frac{(h(1))^n}{n!} M_n(1), \quad (15) \]

This locality is directly responsible for the linked-cluster property, which in turn underlies the extensivity of the thermodynamic functions as \( N \to \infty \) for appropriately regular and short-ranged potentials (Ruelle, 1969).

The above will become clearer as we work out the first few contributions in detail. Using (8), we evaluate,

\[ \frac{\delta W}{\delta v(12)} \bigg|_{v=0} = [-\mathcal{M}_2(12) + \mathcal{M}_1(1) \mathcal{M}_1(2)]_{v=0} = M_1(1) M_1(2), \quad (16) \]

where in the final equality we have used (13) and explicitly noted that \( 1 \neq 2 \). Thus, the first order term in \( W \) is just

\[ \sum_{1,2} M_1(1) v(12) M_1(2) = \frac{1}{2} \sum_{1,2} M_1(1) v(12) M_1(2). \quad (17) \]

Evaluation of the third term in (12) necessitates using eqn (8) twice:

\[ \frac{\delta^2 W}{\delta v(12) \delta v(34)} = \delta \frac{\delta^2 W}{\delta v(34) \delta v(34)} = \frac{\delta^2}{\delta h(1) \delta h(2)} \frac{\delta W}{\delta v(34)} \bigg|_{\bar{v} = 0} \]

\[ + \left[ \frac{\delta^2}{\delta h(1) \delta v(34)} \frac{\delta W}{\delta v(34)} + \frac{\delta^2}{\delta h(2) \delta v(34)} \right] \bigg|_{\bar{v} = 0} \]
\[
\frac{\delta^2 W}{\delta \nu(12) \delta \nu(34)}_{\nu=0} = (\delta(13)\delta(24) + \delta(14)\delta(23))M_2^0(1)M_2^0(2) \\
+ M_1^0(1)M_1^0(3)\delta(24)M_2^0(2) \\
+ M_1^0(1)M_1^0(4)\delta(23)M_2^0(2) \\
+ M_1^0(2)M_1^0(3)\delta(14)M_2^0(1) \\
+ M_1^0(2)M_1^0(4)\delta(13)M_2^0(1).
\] (18)

Thus,

\[
W[h, \nu] = \sum_n M_n^0(1) + \frac{1}{2} \sum_{i, j} M_i^0(1)\nu(12)M_j^0(2) \\
+ \frac{1}{2} \sum_{i, j, k} M_i^0(1)\nu(12)M_j^0(2)\nu(23)M_k^0(3) \\
+ \text{order } \nu^3 \text{ and higher.} \quad (19)
\]

It should be apparent at this point that finding the coefficient of \(\nu^0\) is a trivial but tedious task.

Luckily there is a general method for writing down immediately all terms in the expansion (11) or (19)) for \(W[h, \nu]\). The rule associates the terms of the expansion in a one-to-one manner with a set of linear graphs. After stating the rule and discussing its application, we shall return in Section II.C to its derivation. Before setting down the rule, we must introduce some terminology from graph theory (Essam and Fisher, 1970, see also Domb this Volume, Chapter 1):

**Graphical definitions 1:**

A graph is a set of vertices (points) and edges (lines). Each edge is incident at two distinct vertices.\(^\dagger\) An n-rooted graph, \(n = 0, 1, 2, \ldots\), has \(n\) fixed, distinguishable, external or rooted vertices. All remaining internal vertices are free.

The valence of a vertex is the number of edges incident at that vertex. A vertex of valence \(n\) is called \(n\)-valent.

A connected graph is a graph with the property that any pair of its vertices is joined by a continuous sequence of edges. A graph which is not connected is disconnected.

Two \(n\)-rooted graphs are isomorphic if, when their external vertices are put in one-to-one correspondence, there exists at least one way in which their internal vertices and edges may be placed in one-to-one correspondence in such a way that all connectivity is maintained. The number of distinct ways in which a

\(^\dagger\) "Loops," in which a single edge is incident with both ends at the same vertex, are prohibited.

---

3. Linked cluster expansion

A graph can be made isomorphic to itself is called the symmetry factor\(^\dagger\) \(g\) of the graph. A set of graphs are topologically distinct if no two of them are isomorphic.

![Graphs](image)

**Fig. 1.** The fundamental graphical elements: (a) an edge, (b) an external vertex, (c) an internal vertex, (d) a graph in which the external vertex carries no vertex factor.

When picturing graphs (see Fig. 1), we draw the edges as lines and the external and internal vertices as open and filled circles, respectively. The only exception to this comes in Section II.E and after, where, in the process of

![Graphs](image)

**Fig. 2.** Symmetry factors for the unrooted graphs (a), (b), and (c) are 12, 48, and 24 respectively. The general \(n\)-gon has a symmetry factor \(2n\). The \(n\)-fold multigrid has a symmetry factor \(2n^2\). The complete \(n\)-vertex graph (all pairs connected by a single edge) has a symmetry factor \(n^2\).

In order to calculate \(W[h, \nu]\) one takes the set of all topologically distinct \(0\)-rooted connected graphs. One associates with each graph a contribution according to Rule 1 below, and one sums all such contributions:

**Rule 1: Free Energy \(W\), Unrenormalised Form**

(a) Assign a dummy label to each internal vertex.

(b) For each edge joining vertices \(i\) and \(j\) write a factor \(\nu(ij)\).

(c) For each \(1\)-valent internal vertex \(i\) write a factor \(M_i^0(i)\) (eqn (10), (14)).

(d) For each \(1\)-valent internal vertex \(i\) write a factor \(M_i^0(i)\) (eqn (10), (14)).

(e) For each \(1\)-valent internal vertex \(i\) write a factor \(M_i^0(i)\) (eqn (10), (14)).

(f) For each \(1\)-valent internal vertex \(i\) write a factor \(M_i^0(i)\) (eqn (10), (14)).

(g) For each \(1\)-valent internal vertex \(i\) write a factor \(M_i^0(i)\) (eqn (10), (14)).

(h) For each \(1\)-valent internal vertex \(i\) write a factor \(M_i^0(i)\) (eqn (10), (14)).

(i) For each \(1\)-valent internal vertex \(i\) write a factor \(M_i^0(i)\) (eqn (10), (14)).

(j) For each \(1\)-valent internal vertex \(i\) write a factor \(M_i^0(i)\) (eqn (10), (14)).

(k) For each \(1\)-valent internal vertex \(i\) write a factor \(M_i^0(i)\) (eqn (10), (14)).

(l) For each \(1\)-valent internal vertex \(i\) write a factor \(M_i^0(i)\) (eqn (10), (14)).

(m) For each \(1\)-valent internal vertex \(i\) write a factor \(M_i^0(i)\) (eqn (10), (14)).

(n) For each \(1\)-valent internal vertex \(i\) write a factor \(M_i^0(i)\) (eqn (10), (14)).

(o) For each \(1\)-valent internal vertex \(i\) write a factor \(M_i^0(i)\) (eqn (10), (14)).

(p) For each \(1\)-valent internal vertex \(i\) write a factor \(M_i^0(i)\) (eqn (10), (14)).

(q) For each \(1\)-valent internal vertex \(i\) write a factor \(M_i^0(i)\) (eqn (10), (14)).

(r) For each \(1\)-valent internal vertex \(i\) write a factor \(M_i^0(i)\) (eqn (10), (14)).

(s) For each \(1\)-valent internal vertex \(i\) write a factor \(M_i^0(i)\) (eqn (10), (14)).

(t) For each \(1\)-valent internal vertex \(i\) write a factor \(M_i^0(i)\) (eqn (10), (14)).

(u) For each \(1\)-valent internal vertex \(i\) write a factor \(M_i^0(i)\) (eqn (10), (14)).

(v) For each \(1\)-valent internal vertex \(i\) write a factor \(M_i^0(i)\) (eqn (10), (14)).

(w) For each \(1\)-valent internal vertex \(i\) write a factor \(M_i^0(i)\) (eqn (10), (14)).

(x) For each \(1\)-valent internal vertex \(i\) write a factor \(M_i^0(i)\) (eqn (10), (14)).

(y) For each \(1\)-valent internal vertex \(i\) write a factor \(M_i^0(i)\) (eqn (10), (14)).

(z) For each \(1\)-valent internal vertex \(i\) write a factor \(M_i^0(i)\) (eqn (10), (14)).

\(^\dagger\) This is termed "symmetry number" in Chapter 1. The graphs in the present chapter may contain multiple bonds between vertices which are treated as non-identical.
In this spirit we write,

\[
W[h, v] = \left\{ \begin{array}{l}
\text{sum of all topologically} \\
\text{distinct unrooted connected} \\
\text{graphs according to Rule 1}
\end{array} \right.
\]

\[
= \bullet + \frac{1}{2} \bullet + \frac{1}{2} \bullet + \frac{1}{2} \bullet + \frac{1}{4} \bullet \\
+ \frac{1}{4} \bullet + \frac{1}{4} \bullet + \frac{1}{4} \bullet + \frac{1}{4} \bullet
\]

+ order \( v^4 \) and higher. \quad (20)

The symmetry factor for each graph is given in the form \( 1/g \). The reader will verify that the first four terms of (20) correspond in sequence to the first four terms of (19), according to Rule 1. The remaining terms in (20) give all contributions to \( W \) which are third order in the interaction, i.e., which come from graphs with exactly three edges. Figure 3 gives the contribution to \( W \) of a more complicated graph.

\[ g = 6(2!)^2 = 24 \]

\[
\frac{1}{24} \sum_{1, 2, 3, 4, 5, 6, 7} v(12)v(23)v(14)v(25)v(34)v(47)v(46)v(67)v(56) \\
\times M_3^0(1)M_3^0(2)M_3^0(3)M_3^0(4)M_2^0(5)M_2^0(6)M_3^0(7)
\]

Fig. 3. A 12th order contribution to the Ising free energy according to Rule 1.

Equation (20) gives \( W[h, v] \) for arbitrary inhomogeneous fields and interactions. Although this freedom will be useful in what follows, it is worth pointing out that, if the free energy is all we wish to calculate, considerable simplification is gained by immediately specialising to the translationally invariant case,

\[
h(1) = h, \quad v(12) = V(R_1 - R_2). \quad (21)
\]

The bare semi-invariants \( M_n^0(h) \) are independent of position, and the formal extensivity of \( W \) is realised,

\[
\frac{W}{N} = M_0^0(h) + \left( \frac{1}{2} M_1^0(h) \right)^2 \sum_k V(R) \\
+ \left( \frac{1}{4} M_2^0(h) \right)^2 \sum_k V^2(R) + \left( \frac{1}{2} M_3^0(h) \right)^2 M_2^0(h) \left[ \sum_k V(R) \right]^2 \\
+ \text{order } v^3 \text{ and higher}, \quad (22)
\]

where \( R \) runs over the entire lattice and boundary effects have been neglected (periodic boundary conditions). It is easy to see from (10) and (14) that \( M_n^0(h) \) has parity \( (-1)^n \), so that, when \( h = 0 \), all odd semi-invariants vanish and, of the explicit terms in (22), only the first and third survive.

The most studied example of (22) is when, in addition to (21), the potential acts between nearest-neighbour sites only,

\[
v(12) = \begin{cases} v, & \text{when } 1 \text{ and } 2 \text{ are nearest neighbours,} \\ 0, & \text{otherwise.} \end{cases} \quad (23)
\]

In this case (22) simplifies to

\[
\frac{W}{N} = M_0^0(h) + \frac{q}{2} (M_1^0(h))^2 v + \left[ \frac{q^2}{4} (M_2^0(h))^2 + \frac{q^2}{2} (M_1^0(h))^2 M_2^0(h) \right] v^2 \\
+ \text{order } v^3 \text{ and higher}, \quad (24)
\]

where \( q \), the coordination number of the lattice, is just the number of nearest neighbours of any site. Let us in this case consider a given \( n \)-edged graph \( G_a \) and examine its contribution \( W(G_a) \) to the full free energy. Because of the nearest-neighbour restriction, all terms in the sum required by Rule 1(d) are identical. The number of such terms we write as \( Nm(G_a) \), where \( m(G_a) \) is the free multiplicity of the graph \( G_a \). \( m(G_a) \) measures the number of distinct ways per site of the underlying lattice of which the vertex-labelled graph \( G_a \) can be embedded in the lattice with each vertex assigned to a site of the lattice and each edge lying along a nearest-neighbour bond. In the appendix to this article the free multiplicity is discussed, some of its simple properties are given, and it is related to the weak lattice constants. Jasnow (1969) has tabulated the free multiplicities of 2-rooted graphs for a variety of lattices. It is important to notice that, because the sum in Rule 1(d) is unrestricted, it is quite permissible for graphically distinct vertices to occupy the same lattice site. This is in contrast to the weak and strong lattice constant systems used in other types of expansions and discussed for example by Domb (1960) and by Sykes et al. (1966). (See Domb this Volume, Chapter 1.) The contribution \( W(G_a) \) now is

\[
W(G_a) = \frac{N}{g(G_a)} m(G_a) v^q \left( \prod_{b_n^0} M^0 \right), \quad (25)
\]

where, by the notation \( \prod_{b_n^0} M^0 \), we intend to evoke the product of semi-invariants required for the graph \( G_a \) by Rule 1(c). To find the coefficient of \( v^q \) in the

\[ \text{For a finite lattice with free surfaces } m(G_a) \text{ is not strictly intensive. This remark is not entirely pedantic, since it shows where in the expansion the boundary contribution to } W \text{ may be found. (See Watson, Vol. 1, Chapter 4.) We shall in the text continue to assume periodic boundary conditions, thus guaranteeing intensity of the multiplicity.} \]
expansion for \( W \) we have only to sum up the contributions of all \( n \)-edged graphs. If one is given a list of graphs \( G_n \) along with corresponding symmetry factors and multiplicities, the labour, which is entirely clerical, might be organized as shown in Fig. 4.

<table>
<thead>
<tr>
<th>( G )</th>
<th>( g(G) )</th>
<th>( m(G) )</th>
<th>( W(G)/N )</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image" alt="" /></td>
<td>12</td>
<td>( g )</td>
<td>( \frac{1}{12} q v^3 (M_3^0)^2 )</td>
</tr>
<tr>
<td><img src="image" alt="" /></td>
<td>6</td>
<td>( q^3 )</td>
<td>( \frac{1}{2} q^3 v^3 (M_1^0)^3 M_3^0 )</td>
</tr>
<tr>
<td><img src="image" alt="" /></td>
<td>2</td>
<td>( q^2 )</td>
<td>( \frac{1}{2} q^2 v^3 M_1^0 M_2^0 M_3^0 )</td>
</tr>
<tr>
<td><img src="image" alt="" /></td>
<td>6</td>
<td>( 6p(\delta) )</td>
<td>( p(\delta)v^3 (M_2^0)^3 )</td>
</tr>
<tr>
<td><img src="image" alt="" /></td>
<td>2</td>
<td>( q^3 )</td>
<td>( \frac{1}{2} q^3 v^3 (M_1^0)^2 (M_2^0)^2 )</td>
</tr>
</tbody>
</table>

![Fig. 4](image)

Bookkeeping for the evaluation of the \( v^3 \) term in the nearest-neighbour Ising model free energy. The total \( v^3 \) contribution is the sum of the five terms in the right hand column. \( g \) is the coordination number of the lattice and \( p(\delta) \) is its weak lattice constant for the triangle graph. For loose-packed lattices \( p(\delta) = 0 \). \( p(\delta) = 2, 8 \) on the triangle and f.c.c. lattices, respectively.

So far we have discussed only the free energy expansion. Equations (4)–(6) allow corresponding linked-cluster expansions to be written down for all Ising model cumulant correlations \( \mathcal{M} \) simply by term-by-term differentiation of the free energy. Note that (i) the fields appear in \( W \) only through the semi-invariants \( M_n^0 \) and (ii) differentiation of an \( M_n^0(h) \) has by (14) the very simple effect,

\[
\left( \frac{d}{dh} \right)^1 M_n^0(h) = M_{n+1}^0(h).
\]  

(26)

Consider, for example, differentiation of the first few terms (19) of \( W \):

\[
\frac{\langle s_{11} \rangle}{s} = \langle \mu(1) \rangle = \mathcal{M}_1(1) = \frac{\delta W}{\delta h(1)} = M_1(1)
\]

\[
= M_1^0(1) + \sum \frac{1}{2} M_2^0\nu(12) M_1^0(2)
\]

\[
+ \frac{1}{2} \sum M_2^0\nu(12) M_2^0(2)
\]

(27)

The effect of differentiation is to fix by turn each graphical vertex and to increase by one the order of its bare semi-invariant. When two vertices of the same graph are topologically equivalent, their contributions are, of course, identical.

The result of the above procedure is easily expressed in terms of a graphical rule; however, while we are at it, it will be useful to define a somewhat more general quantity, the full significance of which will only appear in Section II.E. In this spirit we define \( M_n(1) \) the \( n \)th order renormalised semi-invariant,

\[
M_n(1) = \begin{cases} \text{sum of all topologically} \\ \text{distinct 1-rooted connected} \\ \text{graphs according to Rule 2.} \end{cases}
\]  

(28a)

**Rule 2: Renormalised Semi-Invariants, Unrenormalised Form**

(a) Assign the label 1 to the external (root) vertex and a dummy label to each internal vertex.

(b) For each edge joining vertices \( i \) and \( j \) write a factor \( v(ij) \).

(c) For each 1-valent internal vertex \( i \) write a factor \( M_i^0(i) \). For each 1-valent external vertex write a factor \( M_i^0(1) \).

(d) Sum each internal vertex label freely over the entire lattice.

(e) Divide by the symmetry factor of the 1-rooted graph.

The graphical representation (cf. (20)) starts,

\[
M_n(1) = \begin{array}{l}
\text{open circle represents the external vertex 1. Notice that the symmetry} \\
\text{factors for the rooted graphs differ from those of their unrooted analogs.} \\
\text{When } n = 1, \text{ Rule 2 gives the magnetisation (27) of the Ising model.} \\
\text{An additional derivative of (27) gives the pair correlations (5). Note that} \\
\text{there are two types of terms, those in which the } \frac{\delta}{\delta h(2)} \text{ derivative hits the}
\end{array}
\]  

(28b)
already rooted external vertex 1 and those in which it fixes a second internal vertex. The former terms are summed by Rule 2 with \( n = 2 \). Thus,

\[
\mathcal{M}_2(12) = \delta(12)M_2(1) + \left\{ \text{sum of all topologically distinct 2-rooted connected graphs} \right\}
\]

\[
\text{according to Rule 3.}
\]

**Rule 3: Pair Correlations, Unrenormalised Form**

(a) Assign the labels 1 and 2 to the external vertices and dummy labels to the internal vertices.

(b) For each edge joining vertices i and j write a factor \( v(ij) \).

(c) For each l-valent internal vertex i write a factor \( M_1^0(i) \). For each l-valent external vertex \( j = 1, 2 \) write a factor \( M_1^0(1) \).

(d) Sum each internal vertex label freely over the entire lattice.

(e) Divide by the symmetry factor of the 2-rooted graph.

Thus,

\[
\mathcal{M}_2(12) - \delta(12)M_2(1) = \frac{1}{2} \left[ \sum_{\text{2-rooted connected graphs}} \right] + \text{order } v^4 \text{ and higher.}
\]

\[
\text{(30)}
\]

Note that graphs which have the labels of their external vertices interchanged are considered distinct.

Higher order correlations go similarly. In each case multiply differentiated vertices must be counted separately. Thus, for example,

\[
\mathcal{M}_3(123) = \delta(123)M_3(1) + \delta(12)M_{21}(13) + \delta(13)M_{21}(32)
\]

\[
+ \delta(23)M_{21}(21) + \left\{ \text{sum of all topologically distinct 3-rooted connected graphs} \right\}
\]

\[
\text{distinct 3-rooted connected graphs,}
\]

\[
\text{(32)}
\]

where \( M_{21}(ij) \) stands for the sum of all topologically distinct 2-rooted connected graphs by Rule 3 modified for double differentiation at the i vertex.

Equations (20), (28), (30), (31) and their higher order analogs give a recipe for calculating all terms in the Taylor expansions of thermodynamic and correlation functions for the Ising model. Unfortunately the number of contributing graphs in higher orders proliferates very rapidly, so that the unrenormalised linked-cluster expansion is seldom a practical tool. The renormalisations necessary to render it practical will be taken up in Section III.E. Before going on, however, we present (II.C) a proof of the unrenormalised expansions and discuss (II.D) the relation of the unrenormalised linked-cluster expansion to the more conventional weak-embedding expansion for the \( s = \frac{1}{4} \) Ising model. Both these sections may be skipped without destroying the continuity of the development.

C. Proof of the unrenormalised linked-cluster expansion

Proofs of Rule 1 for the unrenormalised linked-cluster expansion for the Ising model free energy have been given by Englert (1963), Bloch and Langer (1965), and Jasnow (1969). Jasnow’s proof is in essence simply a systematisation of the procedure we have used in (16)–(19) to generate the first few orders of the expansion from eqn (8). In what follows we prefer to use the approach of Bloch and Langer, since it is particularly direct and follows the same line as the conventional proofs of the classical-fluid linked-cluster theorem (Huang, 1963; Mayer, 1937; Uhlenbeck and Ford, 1963; Domb, this Volume, Chapter 1).

Direct expansion of the partition function (3) yields:

\[
\exp W[h, v] = Z[h, v] = \text{Tr} \exp \left( \sum \mu(1) M(1) \right) \sum_{n=0}^{\infty} \frac{1}{2^n n!} \left( \sum_{1,2} v(12) \mu(1) \mu(2) \right)^n
\]

\[
= Z_0(h) \sum_{n=0}^{\infty} \frac{1}{2^n n!} \left[ \sum_{1,2 \cdots 2n} v(12) \cdots v(2n-1, 2n) \mu(1) \mu(2n) \right],
\]

\[
\text{(32)}
\]

where \( \langle \rangle \) refers to an expectation value in the \( v = 0 \) ensemble. Expectation values of products such as occur in (32) can always be written in terms of cumulants, e.g.

\[
\langle \mu(1) \mu(2) \rangle = \mathcal{M}_2(12) + \mathcal{M}_2(1), \mathcal{M}_2(2)
\]

\[
\langle \mu(1) \mu(2) \mu(3) \rangle = \mathcal{M}_3(123) + \mathcal{M}_2(12), \mathcal{M}_2(3) + \mathcal{M}_2(13), \mathcal{M}_2(2) + \mathcal{M}_2(23), \mathcal{M}_1(1) + \mathcal{M}_1(1), \mathcal{M}_1(2), \mathcal{M}_1(3).
\]

The general rule is that \( \langle \mu(1) \cdots \mu(2n) \rangle \) is a sum of products of cumulant correlations in which each term corresponds to a partition of the arguments \( (1 \cdots 2n) \) and every possible partition appears once and only once.

The bracketed sum in (32) requires evaluation of \( \langle \mu(1) \cdots \mu(2n) \rangle \) in the \( v = 0 \) ensemble, for which the cumulant correlations \( \mathcal{M}^0 \) contain spatial
δ-functions and bare semi-invariants (13). Because $v(ij) = 0$ when $i = j$, the locality property eliminates from (32) any term in $\langle \mu(1) \ldots \mu(2n) \rangle_0$ in which both ends of the same bond $v(ij)$ have been assigned to the same $\mathcal{M}^0$, i.e., $v(12) \mathcal{M}^0(12\ldots) = 0$. The remaining bracketed quantities can be expressed graphically in the sense of Rule 1 (a)–(d) if we include both connected and disconnected graphs. The $n = 1$ and $n = 2$ brackets are, for example, respectively,

$$[\begin{array}{c}
\vdots
\end{array}] \text{ and } [\begin{array}{c}
\vdots + 4 \vdots + 2 \vdots
\end{array}]$$

(34)

where the numerical factors come from different permutations of the dummy labels. Disconnected contributions are products of connected components. Let us label all topologically distinct connected components by some index $\lambda = 1, 2, \ldots$ and the corresponding contributions according to Rule 1 (a)–(d) by $w_\lambda$. Figure 5 shows how the first few lines of such a listing might look.

<table>
<thead>
<tr>
<th>$\lambda$</th>
<th>$G_\lambda$</th>
<th>$w_\lambda$</th>
</tr>
</thead>
</table>
| 1 | [\begin{array}{c}
\vdots
\end{array}] | $\sum_{1,2} M_1^0(1) v(12) M_1^0(2)$ |
| 2 | [\begin{array}{c}
\vdots
\end{array}] | $\sum_{1,2,3} M_1^0(1) v(12) M_2^0(2) V(23) M_1^0(3)$ |
| 3 | [\begin{array}{c}
\vdots
\end{array}] | $\sum_{1,2} M_2^0(1) v(12)^2 M_2^0(2)$ |

Fig. 5. A partial listing of the contributions of the various connected components in the bracket of eqn (35).

Any term in the bracket is simply a product of one or more $w_\lambda$, $\prod_{\lambda=1}^\infty w_\lambda = n_\lambda$, where $n_\lambda = 0, 1, \ldots$ is the number of times each $G_\lambda$ appears. For example, the terms in (34) are just $[w_1 + 4 w_2 + 2 w_3]$. Note that each term may appear a number of times. This is because the arguments 1, 2, ..., 2n are summed, so contributions in which these arguments have been permuted in such a way as to leave the topology unchanged are identical. The number of such permutations for a graph specified by a given set of $\{n_\lambda\}$ is just

$$2^n n! \prod_{\lambda=1}^\infty \frac{1}{n_\lambda!} g_\lambda^{n_\lambda} =$$

where $g_\lambda$ is the symmetry factor referred to in Rule 1(e). The total contribution to the bracket in (32) of each topology $\{n_\lambda\}$ is just

$$2^n n! \prod_{\lambda=1}^\infty \frac{1}{n_\lambda!} \left( \frac{w_\lambda}{g_\lambda} \right)^{n_\lambda}.$$

(35)

Substitution of (35) into (32) gives

$$W[h, v] = W_0[h] + \sum_{z=1}^\infty \frac{w_z}{z g_z},$$

(36)

which is identical to Rule 1.

The graphical rules for correlation functions may be derived by arguments essentially similar to the above (Englert, 1963). In the evaluation of $\langle X \rangle = \text{Tr} X \exp (-\beta \mathcal{W}) / Z[h, v]$, the denominator divides out all unrooted graphs. The whole procedure is entirely analogous to our treatment of $W$, and we prefer the method of term-by-term differentiation described in II.B.

D. Relation of the linked-cluster and weak-embedding expansions for the free energy

The relation between the linked-cluster and weak-embedding expansions is simple in principle, although, as will be seen in what follows, the enumeration of those terms in one which correspond to a given term in the other can be quite involved. The relation is most easily studied by means of an example. We choose for this purpose the $s = \frac{1}{2}$ Ising model free energy $W$.

The standard weak-embedding expansion (Newell and Montroll, 1953; Domb, 1960) uses the operator identity exp $(\alpha A) = \cosh \alpha + A \sinh \alpha$, valid for any operator $A$ such that $A^2 = 1$, to rewrite the $s = \frac{1}{2}$ Ising partition function (3). Thus,

$$W[h, v] = \sum_T \ln \left[ (2 \cosh h(1)) + \frac{1}{2} \sum_{1,2} \ln \cosh v(12) \right. + \ln 2^{-N} \text{Tr} \left[ \prod_{1,2} (1 + \mu(1) \tanh h(1)) \prod_{1,2} (1 + \mu(1) \mu(2) \tanh v(12)) \right].$$

(37)

where $\prod_{(1,2)}$ denotes the product over all pairs of sites. Development of the trace in powers of $\tanh v$ yields the weak-embedding expansion. We maintain as individually variable the local fields and bond strengths in order to facilitate detailed comparison with the linked-cluster form of the development. Terms which survive the trace must have an even number of factors $\mu(i)$ at each site $i$ and, thus, can be designated uniquely by listing the contributing bonds $v(ij)$. The topology of the contributing bonds constitutes a graph. Both connected and disconnected graphs appear. When the logarithm is taken, all those parts of the disconnected contributions which go as $N^2$, $n > 1$,
cancel against iterations of lower orders, thus guaranteeing extensivity in the thermodynamic limit.

The first few terms in the resulting expression are shown in equation (38):

\[ W[h, v] - W_0[h] = \frac{1}{2} \sum_{i, 2} \ln \cosh v(12) \]
\[ + \frac{1}{2} \sum_{i \neq 3} \tanh h(1) \tanh v(12) \tanh h(2) \]
\[ + \frac{1}{2} \sum_{i \neq 3} \tanh^2 h(1) \tanh v(12) \tanh^2 h(2) \]
\[ + \frac{1}{2} \sum_{i \neq 3} \tanh h(1) \tanh v(12) \tanh^2 h(2) \tanh v(23) \tanh h(3) \]
\[ + ... \]

where we have indicated the graph corresponding to each term in the weak-embedding sense. Each edge \( i, j \) carries a factor \( \tanh v(ij) \). Each vertex \( i \) with odd valence carries a factor \( \tanh h(i) \). The disconnected graphs come from the expansion of the logarithm.

On the other hand, the bare semi-invariants (14) for the linked-cluster expansion are for \( s = 1/2 \),

\[ M^0_a(h) = \frac{d^n}{dh^n} \ln (2 \cosh h), \]

\[ M^0_1 = \tanh h, \quad M^0_2 = 1 - \tanh^2 h, ... . \] (39)

Substitution into (19) gives,

\[ W[h, v] - W_0[h] = \frac{1}{2} \sum_{i, 2} \tanh h(1)v(12) \tanh h(2) \]
\[ + \frac{1}{2} \sum_{i, 2} (1 - \tanh^2 h(1))v(12)(1 - \tanh^2 h(2)) \]
\[ + \frac{1}{2} \sum_{i, 2, 3} \tanh h(1)v(12)(1 - \tanh^2 h(2))v(23) \tanh h(3) + ... \]
\[ = \frac{1}{2} + \frac{1}{4} + \frac{1}{4} + ... \] (40)

To compare (38) and (40), it is necessary (i) to expand \( \ln \cosh v \) and \( \tanh v \) in powers of \( v \) and (ii) to dissect out of the free linked-cluster sums those contributions from each set of distinct bonds. The connections in Fig. 6 show which set of graphs in one expansion contribute to a given term of the other.

Note that each weak graph will, in a complete tabulation, contribute to an infinite number of linked-cluster graphs (since \( \tanh v \) has all odd powers of \( v \)), while each linked-cluster graph contributes only to a finite number of weak graphs (with the same number of lines or fewer).

Fig. 6. Graphical correspondences between the linked-cluster and weak-embedding expansions for the \( s = 1/2 \) Ising free energy. Connections show which graphs in one expansion contribute to a given term in the other.

To clarify this relation it is useful to sort the terms of both expansions according to which connected set of bonds \( \{v(ij)\} \) is used. This sorting according to a physical cluster of bonds has been discussed by Rushbrooke and Morgan (Rushbrooke and Morgan, 1961; Morgan and Rushbrooke, 1961; Rushbrooke, 1964), Elliott and Heap (Elliott and Heap, 1962; Heap, 1963), Jasnow and Wortis (1967), and others. Such a physical cluster receives on the one hand contributions from all linked-cluster graphs which can be embedded in it using every physical bond at least once (note that the free sums allow multiple usage of each site and bond—quite complicated graphs can be “collapsed” to fit into simple physical clusters) and on the other hand contributions from all weak graphs which can be embedded in it using every bond once and only once. A further sorting of these correspondences by powers of \( v(ij) \) for each bond extends Fig. 6 as far as patience permits.

The complexity of the interrelation between the two types of expansion rests—in a language restricted to the nearest-neighbour case (23)—on the connection between the free multiplicities \( m(G) \) defined after (24) and the weak lattice constants. This connection, which is touched upon in the appendix, has not yet been seriously explored.

E. Vertex renormalisation: the correlations

To make the linked-cluster expansion practical from a calculational point of view, one must find a way of reducing the number of contributing graphs.
This is done by selective resummation of classes of graphs. The effect is to introduce a degree of implicitness into the procedure and thus to exchange topological complexity for algebraic complexity.

![Graphs](image)

**Disassembly of a Vertex**†

A vertex $V$ of a graph $G$ is disassembled by the following procedure:

(i) Clip away all edges from $V$ (thereby dividing $G$ into a number of disconnected parts).

(ii) Reattach to $V$ all clipped edges belonging to disconnected parts containing external vertices.

(iii) Join to one another the clipped edge ends belonging to each additional connected part (if any).

This process is pictured for several graphs in Fig. 9.

![Disassembly Graphs](image)

**Graphical Definitions II**

The unrooted parts formed in the process of disassembly are called 1-insertions. The clipped vertex of a 1-insertion will be regarded as the external vertex of the 1-insertion and will be drawn without a circle.‡

An articulation point of a rooted graph is a vertex the disassembly of which produces at least one 1-insertion. An articulation point of an unrooted graph is a vertex the disassembly of which produces at least two 1-insertions.

A graph which contains no articulation points is 1-irreducible. A graph which contains one or more articulation points is 1-reducible.

The 1-skeleton of a rooted graph is the graph produced by disassembling in turn all vertices of the graph and discarding all 1-insertions thereby produced.

† This operation differs, for example, from deletion of a vertex, which removes all incident edges (Essam and Fisher, 1970), in that no graphical elements are gained or lost. From the algebraic point of view, we are simply regrouping the factors in each perturbation theoretic term. This is the origin of the slight differences which will appear between our terminology and that of Essam and Fisher.

‡ This notation is intended to suggest that such a vertex carries no semi-invariant factor.
Any rooted graph has a unique 1-irreducible 1-skeleton, as illustrated in Fig. 7, to which it can be reduced by clipping away all 1-insertions. (Note that the open circle is the 1-skeleton of every 1-rooted graph.) Conversely any rooted graph can be constructed from a 1-irreducible 1-skeleton in a unique way by appending appropriate combinations of 1-insertions at each skeletal vertex.†

Because of the free sums in parts (d) of Rules 1–3, each 1-insertion enters as a factor in the overall graphical contribution. To keep track of the appropriate subscript on the bare semi-invariant, it is necessary to classify 1-insertions according to the valence of the external vertex. We therefore define the self-field \( G_n(1) \) as,

\[
G_n(1) = \left\{ \begin{array}{l}
\text{sum of all topologically} \\
\text{distinct } n\text{-valent 1-insertions} \\
\text{according to Rule 4}
\end{array} \right.
\]

(41a)

**Rule 4:** Self-Field, Unrenormalised Form

(a) Assign the label 1 to the external vertex and a dummy label to each internal vertex.

(b) For each edge joining vertices i and j write a factor \( \psi(ij) \).

(c) For each 1-valent internal vertex i write a factor \( M_s^0(i) \). For the external vertex write a factor 1.

(d) Sum each internal vertex label freely over the entire lattice.

(e) Divide by the symmetry factor of the 1-insertion.

In this form \( G_n \) depends on \( \psi \) and \( h \) (via the \( M_s^0(\cdot) \)'s). The graphical representation of the first few \( G_n \)'s looks like:

\[
G_1(1) = \\
G_2(2) = \\
G_3(1) = \frac{1}{2}
\]

order \( \psi^4 \) and higher.

(41b)

The factors \( G_n \) play the physical role of a generalized 1-body effective field. They have a parallel in the classical-fluid expansion (see II.F), and are closely analogous to the quantum-mechanical self-energy operator \( \Sigma \) (Kadanoff and Baym, 1962).

We are now in a position to calculate the net contribution of all possible
decorations of a single given skeletal vertex, as pictured for example in Fig. 8. The presence of \( k \) identical 1-insertions at the same vertex makes a multiplicative contribution of \( k! \) to the overall symmetry factor for the decoration of an \( n \)-valent skeletal vertex:

\[
M_n(1) = M_n^0(1) + \sum_{i=1}^{\infty} G_i(1) M_{n+i}(1) + \frac{1}{2} \sum_{i, j=1}^{\infty} G_i(1) G_j(1) M_{n+i+j+m}(1) + \ldots
\]

\[
= \left[ \exp \sum_{i=1}^{\infty} G_i(1) \frac{\partial}{\partial \Omega} \right] M_n^0[1; \partial]_{\Omega = h(1)},
\]

with \( n = 1, 2, 3, \ldots \), which is a re-expression of (28) and includes the magnetisation \( M_s(1) = M_1(1) \) as a special case.†

**Summation of all rooted graphs having the same 1-skeleton is now accomplished by the replacement** \( M_s^0 \rightarrow M_s \) **at the skeletal vertices.** The only difficulty in passing from (42) to the above statement is the question of symmetry factors. Suppose a given rooted graph \( G \) is composed of a 1-skeleton, \( G_s \), decorated by a series of 1-insertions \( G_{11}, G_{12}, \ldots \). The symmetry factor \( g(G) \) is composed of several factors,

\[
F_{SV} = \frac{1}{g(G)} \frac{1}{\Pi g(G_j)} \frac{1}{F_{SV}^0}
\]

(43)

Where \( F_{SV} (SV = \text{single vertex}) \) stands for the combinatorial factors arising from the presence of identical 1-insertions at a single vertex. \( F_{SV} (EV = \text{equivalent vertex}) \) stands for the combinatorial factors by which the skeletal symmetry factor \( g(G_j) \) is reduced due to distinct decoration of previously equivalent skeletal vertices. For example, for the graph of Fig. 7, \( g(G_2) = 4, \Pi g(G_j) = 2^3 = 4, F_{SV} = 3! = 6, F_{SV}^0 = 2, \) and \( g(G) = 48. \) In the renormalised form only the factor \( 1/g(G_j) \) is explicit. The \( g(G_j) \) are absorbed in the self-fields; the \( F_{SV} \) are incorporated in the exponential form of (42); and, the \( F_{SV}^0 \) are supplied by equivalent cross-terms in the expansion of the product of renormalised semi-invariants.

The procedure for finding the vertex renormalised form of a bare expansion is to group all contributing graphs with the same 1-skeleton and to sum them by putting \( M_s^0 \rightarrow M_s \). For example, the two-point part of the pair correlations given by (29), (30), and Rule 3 may be re-expressed as,

\[
	o_{20} = \delta(12) M_2(1) + \left\{ \begin{array}{l}
\text{sum of all topologically distinct} \\
\text{2-rooted 1-irreducible connected} \\
\text{graphs according to Rule 5}
\end{array} \right.
\]

(44)

† Equation (42) is the classical analog of the quantum many-body Dyson equation (Kadanoff and Baym, 1962). \( M_s^0 \) corresponds to the bare propagator \( G_0 \) and \( M_s \) corresponds to the renormalised propagator \( G \). The fact that \( M_s^0 \) and \( M_s \) are spatially local reflects the locality of the Hamiltonian (1) in the absence of interaction.
Rule 5: Pair Correlations, Vertex Renormalised Form
(a) Assign labels 1 and 2 to the external vertices and dummy labels to the internal vertices.
(b) For each edge joining vertices i and j write a factor \( v(ij) \).
(c) For each 1-valent internal vertex i write a factor \( M_i(i) \). For each 1-valent external vertex \( j = 1, 2 \) write a factor \( M_{1+1}(i) \).
(d) Sum each internal vertex label freely over the entire lattice.
(e) Divide by the symmetry factor of the 2-rooted graph.

Graphically,
\[
M_2(12) - \delta(12)M_2(1) = \begin{array}{c}
\text{Graphical representation of } M_2(12) - \delta(12)M_2(1) \text{ with vertex labels and edge factors.}
\end{array}
\]

Equation (45) sums an infinite number of terms in the unrenormalised expansion and is exact through order \( v^3 \) with fewer graphs than the corresponding bare expression (30). The simplification is even more impressive in higher orders.

In contrast to the bare expansion, for which the vertex factors \( M_n^0 \) are known directly (see (10) and (14)), the renormalised expansion is only useful after the semi-invariants \( M_n^* \) have been calculated (e.g. from (41) and (42)). This is facilitated by using a renormalised expression for the self-fields \( G_n \):
\[
G_n(1) = \left\{ \begin{array}{l}
\text{sum of all topologically distinct } n \text{-irreducible} \\
\text{1-insertions which are } n \text{-valent at the external vertex according to Rule 6.}
\end{array} \right.
\]

Rule 6: Self-Field, Vertex Renormalised Form
Same as Rule 4 except:
(c) For each 1-valent internal vertex i write a factor \( M_i(i) \). For the external vertex write a factor 1.

\[
\begin{align*}
G_2(1) & = \frac{1}{2} + \frac{1}{2} + \frac{1}{2} + \frac{1}{2} + \text{order } v^4 \text{ and higher,} \\
G_3(1) & = \frac{1}{6} \left( \text{exact} \right) + \frac{1}{2} + \text{order } v^5 \text{ and higher.}
\end{align*}
\]

In this form the self-field depends functionally on \( v \) and the set \( M_n, n = 1, 2, \ldots \).
Thus, \( G(1) = G[1; M, v] \), and (42) becomes a non-linear equation, schematically,
\[
M = \exp \left( G[M, v] \right) M^0 \quad \text{or, more symmetrically,} \quad M^0 = \exp \left( -G[M, v] \right) M,
\]
which can in principle be inverted to give \( M^0, v \). Once the \( M_i \)'s are known as functions of the variables \( h \) and \( v \), then eqns (44) and (45) and their higher-order analogues evaluate the cumulant correlations.

In the derivation of high-temperature series expansions (Jasnow, 1969; Jasnow and Wortis, 1968) eqns (47) and (48) are solved iteratively in powers of \( v \). To zeroth order \( M_n = M_n^0 \), which are given by (10) and (14). Note that \( G_n \sim v^n \). Once the \( M_n^* \)'s are known to order \( v^4 \), gives the \( G_i \)'s to order \( l + 1 \). These new \( G_i \)'s give the \( M_n^* \)'s to order \( l + 1 \), and so on. Stanley (1967) lists all \( h = 0 \) \( M_2 \) graphs necessary through order \( v^8 \) (close-packed lattices) and \( v^9 \) (loose-packed lattices).

To go beyond iteration, it is necessary to use other methods (such as those discussed in Section I.I.H) to find \( G[M, v] \). Inverting (48) may be facilitated by forming the Fourier transforms of the bare semi-invariants,
\[
M_n^0(h) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ikx} M_n^0(k),
\]
where some care must be taken for \( n = 0, 1 \). Then, from (42),
\[
M_n(h) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \left( \exp \sum_{i=1}^{\infty} (ik)^l G_i[M, v] \right) e^{ikx} M_n^0(k),
\]
In the translationally invariant situation (21), (50) is a set of coupled algebraic equations for the numbers \( M_n, n = 1, 2, \ldots \).

F. Vertex renormalisation: the free energy
Free energy graphs are unrooted and hence have no unique 1-skeleton. The direct regrouping described in Section I.I.E is therefore inapplicable. This obstacle can be circumvented by two routes. De Dominicis (1962), Englert (1963), and Bloch and Langer (1965) use a topological method. Following an earlier publication (Wortis, et al., 1969), we prefer simply to integrate eqn (4),
\[
M_i(1) = \frac{\delta W[h, v]}{\delta h(1)},
\]
subject to the boundary condition that, as \( h(1) \rightarrow \infty \), the only contributing state is \( \mu(1) = 1 \) for all sites 1. Thus, \( M_1^0(1) = 1, M_n^0(1) = 0, n > 1 \), and only the first two terms in (29) are non-vanishing, with analogous simpli-
fifications for other quantities: as $h(1) \to \infty$ for all sites $1$,
\[
W = \sum_1 h(1) + \frac{1}{2} \sum_{1,2} v(12),
\]
\[
M_1(1) = 1, \quad G_1(1) = \sum_1 v(12),
\]
\[
M_n(1) = G_n(1) = 0 \text{ for } n > 1.
\] (52)

Equation (42) with $n = 1$ provides a vertex renormalised expression for $M_1(1)$. Our task is to construct a functional $W$ which satisfies (51) subject to (52).

Naively, it might seem that a good candidate for $W$ would be $\Sigma_1 M_0(1)$, with $M_0(1)$ defined by (42) with $n = 0$. On closer inspection we note that $G_n$ depends on $h$ through the renormalised semi-invariants $G[M(h), v]$. Thus, direct differentiation of (42) gives
\[
\frac{\delta}{\delta h(1)} \sum_2 M_0(2) = M_1(1) + \sum_2 \sum_{n=1} G_n(2) \frac{\delta G_n(2)}{\delta h(1)} M_n(2).
\] (53)

Another appealing candidate is the symmetrical quantity,
\[
\Phi[M, v] = \left\{ \text{sum of all topologically distinct 1-irreducible 0-rooted graphs} \right\} \text{ according to Rule 7}.
\] (54)

Rule 7: The Functional $\Phi$, Vertex Renormalised Form
Same as Rule 1 except:
(c) For each 1-valent internal vertex $i$ write a factor $M_i(i)$.

\[
\phi[M, v] = \frac{1}{2} \sum_{1,2} v(12) M_1(1) + \sum_{n=1} G_n(2) \frac{\delta G_n(2)}{\delta h(1)} M_n(2).
\] (55)

$\Phi$, which is like a thermodynamic potential, has as its natural variables $v$ and the renormalised semi-invariants. It is easy to verify that
\[
\frac{\delta \Phi[M, v]}{\delta M_0(1)} = G_0(1).
\] (56)

For example, consider the first term of (55):
\[
\frac{1}{2} \sum_{1,2} M_1(2) v(12) M_1(1).
\] (57)

Differentiation of (57) with respect to $M_1(1)$ yields $G_1(1) = \Sigma_2 v(12) M_1(2)$. (Note that (57) is the only 1-irreducible graph containing a 1-valent vertex.) In general, term-by-term differentiation of (55) leads directly to (47). The

\* The single vertex is specifically omitted from this sum.

only point requiring comment is the symmetry factors. It suffices to note that, in the differentiation (56), vertices in (55) equivalent under symmetry operations of the graph contribute additively. The factor thus produced serves to lower the symmetry factor of the unrooted graph to that of the 1-rooted graph as required by Rule 6(e).

What is the field derivative of $\Phi$? Use of (56) and the chain rule gives,
\[
\frac{\delta \Phi}{\delta h(1)} = \sum_2 \sum_{n=1} \frac{\delta \Phi}{\delta M_n(2)} \frac{\delta M_n(2)}{\delta h(1)} = \sum_2 \sum_{n=1} G_n(2) \frac{\delta M_n(2)}{\delta h(1)}.
\] (58)

The sum of (53) and (58) yields,
\[
\frac{\delta}{\delta h(1)} \left[ \sum_2 M_0(2) + \Phi \right] = M_1(1) + \frac{\delta}{\delta h(1)} \left[ \sum_2 \sum_{n=1} G_n(2) M_n(2) \right].
\] (59)

Thus,
\[
W = \sum_2 M_0(2) + \Phi - \sum_2 \sum_{n=1} G_n(2) M_n(2),
\] (60)

which can easily be shown to satisfy (52). When once the renormalised semi-invariants have been computed (as discussed in II.E), then (60) evaluates the free energy.

If properly interpreted, (60) has an interesting stationarity property. Consider the functional
\[
\mathcal{W}_1[M, v, h] \equiv \sum_2 \left[ \left( \exp \sum_{n=1} \frac{G_n(2)}{h} M_n(1) \right) \left| \frac{\partial}{\partial h(1)} \right| \right]_{h=n(2)},
\]
\[
+ \Phi[M, v] - \sum_2 \sum_{n=1} G_n(2) M_n(2),
\] (61)

which is equal to $W$ provided the $M_n, n \geq 1$, are related to the fields $h$ via (42). We choose to regard $\mathcal{W}_1$ as depending separately on the $M_n$'s, $n \geq 1$, (via $\Phi[M, v]$ and $G[M, v]$) and the fields $h$ which appear explicitly in the $M_n$'s of first term on the right. Direct differentiation of (61) using (56) gives,
\[
\frac{\delta \mathcal{W}_1}{\delta M_1(1)} \bigg|_{h \text{ fixed}} = \sum_2 \sum_{n=1} \frac{\delta^2 \Phi}{\delta M_n(2)} M_n(2),
\] (62)

so that the physical free energy $W$ is a stationary point of $\mathcal{W}_1$. An additional derivative of (62) shows that the stationary point is not necessarily an extremum.

There is another related variational principle (Bloch and Langer, 1965) which can be proved to be a maximum principle. The free energy $W[h, v]$ is
ultimately a functional of the inhomogeneous applied magnetic field $h$. We are free, equivalently, to regard $W$ as functional of the inhomogeneous magnetisation $M_1$ via the dependence $W[h[M_1, v], v]$ provided that the magnetisation $M_1 = M_1[h, v]$ is invertible. This will be so, provided that the Jacobian connecting $M_1$ and $h$ is non-vanishing, which in turn is proved by the observation that the real symmetrical fluctuation matrix,

$$\frac{\delta M_1(1)}{\delta h(2)} = \frac{\delta^2 W}{\delta h(1) \delta h(2)} = \langle (\mu(1) - \langle \mu(1) \rangle)(\mu(2) - \langle \mu(2) \rangle) \rangle,$$  

is positive definite. The generator of the Legendre transformation to the variables $[M_1, v]$ is,

$$\Psi[M_1, v] \equiv W[h[M_1, v], v] - \sum_2 h[2; M_1, v]M_1(2),$$

with

$$\frac{\delta \Psi}{\delta M_1(1)} = \sum_2 \frac{\delta W}{\delta h(2)} \frac{\delta h(2)}{\delta M_1(1)} - \sum_2 \frac{\delta h(2)}{\delta M_1(1)} M_1(2) - h_1(1) = - h[1; M_1, v].$$

(64)

Notice that

$$- \frac{\delta^2 \Psi}{\delta M_1(1) \delta M_1(2)} = \frac{\delta h[1; M_1, v]}{\delta M_1(2)}$$

is the inverse of (63) and, therefore, positive definite. The functional,

$$\mathcal{W}_2[M_1, v; h] \equiv \Psi[M_1, v] + \sum_1 h(1)M_1(1),$$

(65)

(as in (61) the field $h$ is to be regarded as a parameter) has the property that it is a maximum and equal to the physical free energy $W$ when $M_1$ is put equal to the physical magnetisation distribution corresponding to the field $h$.

The functional $\mathcal{W}_2$ is asymmetrical in the renormalised semi-invariants because of the special relationship (4) between $h$ and $M_1$. By defining a set of fictitious fields (Bloch and Langer, 1965; Wortis et al., 1969) related to the higher-order semi-invariants as $h$ is to $M_1$, it is possible to define an entirely symmetrical generalisation of $\mathcal{W}_2$, which is stationary under variations of all $M_n$'s, $n \geq 1$, but, unfortunately, not maximal.

G. The classical-fluid linked-cluster expansion as a special case

It is not our purpose in this section to review the extensive literature on the classical fluid (De Dominicis, 1962; Stell, 1964). Rather, we wish to sketch the classical-fluid linked-cluster development only sufficiently so that the reader familiar with the classical situation will appreciate the very close parallel with the present development. Skipping this section will not destroy the continuity of the text.

It is convenient to introduce a single-particle potential field $u(r)$, which plays a role analogous to that of the magnetic field $h$. The Hamiltonian for $N$ particles can then be written,

$$- \beta \mathcal{W}_N = \sum_{i=1}^N \left( - \frac{p_i^2}{2m} + u(r_i) \right) + \sum_{(ij)} v(r_i - r_j),$$

(66)

where all energies are in units of $kT$ and we have chosen $u$ and $v$ positive when they tend to bind. All momentum integrals are trivial and the grand partition function is written (Huang, 1963),

$$\Xi[u, v] = \sum_{N=0}^\infty \frac{z^N}{N!} \int (dr_1) \cdots (dr_N) \exp \left[ \sum_{i=1}^N u(r_i) + \sum_{(ij)} v(r_i - r_j) \right],$$

(67)

where $z$ is the fugacity $e^{\mu/\lambda_d}$ ($\mu =$ chemical potential, $\lambda =$ thermal wavelength, $d =$ dimensionality). In analogy to (3) we write

$$W[u, v] = \ln \Xi.$$

(68)

The connection with thermodynamics is $\beta PV = \ln \Xi$, where $P$ is the pressure and $V$, the volume. The usual $n$-particle distribution functions are,†

$$\rho_n(r_1, \ldots, r_n) \equiv \rho_n(1 \ldots n)$$

$$= \frac{1}{N!} \sum_{(i-n)} \frac{1}{(i-n)!} \int (dr_{n+1}) \cdots (dr_N) \exp \left[ \sum_{i=1}^N u(r_i) + \sum_{(ij)} v(r_i - r_j) \right]$$

(69)

which may be generated by differentiation,

$$\frac{1}{\Xi} \frac{\delta \Xi}{\delta u(1)} = \rho_1(1), \quad \frac{1}{\Xi} \frac{\delta^2 \Xi}{\delta u(1) \delta u(2)} = \rho_2(12) + \delta(12) \rho_1(1), \text{etc.}$$

Clustering functions $U$ may be derived by direct differentiation of $W$,

$$U_n(1 \ldots n) \equiv \frac{\delta^W}{\delta u(1) \ldots \delta u(n)},$$

(70)

which are the analogs of our $\mathcal{U}_n(1 \ldots n)$ of (6) and differ from the usual Ursell functions $U_n$ (Stell, 1964) by the presence of $\delta$-functions, e.g.,

$$U_2(12) \equiv \frac{\delta^2 W}{\delta u(1) \delta u(2)} = \rho_2(12) - \rho_1(1) \rho_1(2) + \delta(12) \rho_1(1)$$

$$= U_2(12) + \delta(12) \rho_1(1).$$

† Functional differentiation with respect to a continuous function at a point requires a little discussion (Morita and Hiroike, 1961a, b; Volterra, 1959; Berezin, 1966). Since this discussion is entirely irrelevant to our main purposes, we simply remark that the concerned reader may henceforth imagine himself to be dealing with a gas confined to a lattice.
The non-interacting free energy is (cf. (9)):

$$W_0[u] = W[u, v = 0] = \int (dr) M_0^0(r) = z \int (dr) e^{\nu(r)},$$  \hspace{1cm} (71)

from which it follows that (cf. 14),

$$M_n^0(r) = z e^{\nu(r)} \text{ for all } n = 0, 1, 2, \ldots.$$  \hspace{1cm} (72)

By choosing \( n = 1 \) and comparing with (69), \( z e^{\nu(r)} \) may be identified with \( \rho_1^0(r) \), the non-interacting particle density. The unrenormalised rule for the free energy may now be derived just as in Sections II.B or II.C. Everything is exactly the same except that the unrenormalised semi-invariants are given by (72) in place of (10) and (14). To compute the difference \( (W[u, v] - W_0[u, v]) \), one sums all topologically distinct unrooted connected graphs according to (cf. Rule 1):

Rule 8A: Classical-Fluid Free Energy \( W \), Unrenormalised \( \nu \)-form

(a) Assign a dummy label to each internal vertex.

(b) For each edge joining vertices \( i \) and \( j \) write a factor \( \nu(ij) \).

(c) For each vertex \( i \) write a factor \( z e^{\nu(i)} = \rho_1^0(i) \).

(d) Integrate each internal vertex label freely over the volume of the container.

(e) Divide by the symmetry factor of the unrooted graph.

Equation (20) gives the first few terms of the sum.

The important difference between Rule 8A and Rule 1 is in part (c), where Rule 8A requires a vertex factor \( \rho_1^0(i) \) independent of valence. This valence-independence, which follows directly from the exponential form of \( M_0^0 \) (eqn (72)), is the only important respect in which the magnetic expansion differs from the classical-fluid expansion. This difference produces a number of simplifications.

The reader will have noticed that the expansion given by Rule 8A is in terms directly of the pair potential rather than of the Mayer \( f \)-function, \( f(12) = (e^{\nu(12)} - 1) \). To obtain the traditional form we sum over multiedges:

$$f(12) = 1 + \frac{1}{2} \left\{ \frac{1}{3} \right\} + \frac{1}{4} \left\{ \frac{1}{6} \right\} + \ldots.$$  \hspace{1cm} (73)

Note that each edge of multiplicity \( n \) contributes to the symmetry factor \( g \) a factor \( n! \). By omitting the vertex circles in (73), we wish to emphasise that \( f \) contains none of the vertex factors 8A(c). We now group together in a class all graphs contributing to 8A which differ only in the degree of multiplicity of corresponding edges. The replacement \( \nu(12) \rightarrow f(12) \) sums each such class, producing the familiar result that to calculate \( (W[u, v] - W_0[u, v]) \) one may sum all topologically distinct unrooted connected graphs with no multiedges according to:

Rule 8B: Classical-Fluid Free Energy \( W \), Unrenormalised \( f \)-form

Same as Rule 8A except:

(b) For each edge joining vertices \( i \) and \( j \) write a factor \( f(ij) = (e^{\nu(i)} - 1) \).

The first few terms in this form of the expansion are (cf. (20)),

$$W[u, f] - W_0[u] = \frac{1}{2} \left( \frac{1}{3} \right) + \frac{1}{2} \left( \frac{1}{6} \right) + \ldots.$$  \hspace{1cm} (74)

Note that the summation over graphs differing only with respect to edge multiplicity cannot be done in the magnetic case, since each level of multiplicity requires a different vertex factor \( M_n^0 \) due to the changed valence.

Vertex renormalization goes through just as before. Because the vertex factors \( M_n^0 \) are valence-independent, there is no need to classify the self-fields \( G_n \) according to their external valence. The renormalised vertex is just the local density \( \rho_1^0 \) (cf. the identification \( M_1^0 = M_2^0 \)) and the local magnetisation, after (42)). The self-field \( G(1) \) is therefore (cf. Rule 6 and eqn (46)),

$$G(1) = \left\{ \begin{array}{c}
\text{sum of all topologically distinct} \\
\text{1-irreducible 1-insertions with} \\
\text{no multiedges according to Rule 9.}
\end{array} \right\}$$  \hspace{1cm} (75)

Rule 9: Classical-Fluid Self-field, Vertex Renormalized \( f \)-form

(a) Assign the label 1 to the external vertex and a dummy label to each internal vertex.

(b) For each edge joining vertices \( i \) and \( j \) write a factor \( f(ij) = (e^{\nu(i)} - 1) \).

(c) For each internal vertex \( i \) write a factor \( \rho_1^0(i) \). For the external vertex write a factor 1.

(d) Integrate each internal vertex label freely over the volume of the container.

(e) Divide by the symmetry factor of the 1-insertion.

The first few terms are:

$$G(1) = 1 + \frac{1}{2} \left\{ \frac{1}{3} \right\} + \frac{1}{2} \left\{ \frac{1}{6} \right\} + \ldots + \text{order } f^5 \text{ and higher.}$$  \hspace{1cm} (76)

Of course, corresponding expressions in terms of \( v \) rather than \( f \) or in terms of the unrenormalised vertex \( \rho_1^0 \) (cf. Rule 4) could also be written down.
The analog of (42), expressing the decoration of an unrenormalised vertex is simply,

$$\rho_1(1) = e^{\omega(1)} \rho_1^0(1). \quad (77)$$

Note the absence of derivatives. The vertex renormalised free energy is given by (cf. (60)),

$$W = \int (dr_1) \rho_1(1) + \Phi - \int (dr_2) G(1) \rho_1(1), \quad (78)$$

where, in terms of the Mayer f-function, $\Phi$ is given by the sum of all topologically distinct connected 1-irreducible unrooted graphs with no multiedges according to Rule 10 (cf. Rule 7):

**Rule 10: Classical-Fluid Functional $\Phi$, Vertex Renormalised f-form.**

Same as Rule 9 except:

(c) Divide by the symmetry of the unrooted graph.

Rules 9 and 10 give $\Phi$ and $G$ as functions of the particle density $\rho_1$. In the translationally invariant situation $u(1) = 0$, $v(12) = v(r_1 - r_2)$, (78) may be expanded in powers of the density. Graphs with exactly $n$ vertices contribute to $\rho_1^n$. Thus,

$$\beta P = \frac{W}{V} = \rho_1 + \frac{\Phi}{V} - \rho_1 G$$

$$= \rho_1 + \frac{\rho_1^2}{2} \int (dr) f(r) - \frac{\rho_1^3}{3} \int (dr_1)(dr_2)(fr_1)fr_2f(r_1 - r_2) + \text{order } \rho_1^4 \text{ and higher.} \quad (79)$$

which is just the ordinary virial expansion.

H. $\Phi$-Derivable approximations

Despite renormalisation, the series expansions always involve an infinite number of terms. When there is a small expansion parameter (e.g. $v$ or $\rho_1$), then it may be that only a finite number of terms contribute appreciably. On the other hand, there are situations where it is convenient to have an analytic solution for the free energy, correlations, etc., which is at least qualitatively valid over a wide range of parameters. Such solutions must sum an infinite subset of perturbation theory graphs. Which subset to choose is dictated by an understanding of the physics. So far it has not been possible to pick out an analytically summable subset of graphs which gives proper critical behaviour; however, these closed-form approximations are of sufficient historical interest and sufficient practical importance in non-critical regions that they deserve mention.

We shall not attempt to review the history of approximate solutions to the Ising model (Newell and Montroll, 1953; Brush, 1967; see also Burley Volume 2, Chapter 9). Rather we limit ourselves to the presentation of a certain class of those solutions which are closely related to the development of Sections II.E and II.F and which are complete and internally consistent in a sense which will be made clear below.

The basic philosophy of the $\Phi$-derivable approximations (Baym, 1962; Bloch and Langer, 1965) is that they involve direct approximation for the free energy functional in the presence of arbitrary inhomogeneous fields $h$. Thus, corresponding approximations to all correlation functions may be obtained from

$$\langle \mathcal{M}_n(1 \ldots n) \rangle_{\text{approx}} = \frac{\delta \langle W \rangle_{\text{approx}}}{\delta h(1) \ldots \delta h(n)}, \quad (80)$$

with the guarantee that, being related to the same underlying free energy, they will all have singular behaviour at the same points and obey certain self-consistency conditions such as the well-known susceptibility sum rule,

$$N_X = \frac{\Delta^2 W}{\Delta h^2} = \sum \mathcal{M}_2(12). \quad (81)$$

The procedure is as follows:

Step (a): Choose an approximate $\overline{\Phi}[\bar{M}, v]$ consisting of a subset of the terms of (55) (Rule 7). The approximate free energy $\overline{W}[\bar{M}, v]$ is given by (60):

$$\overline{W}[\bar{M}, v] = \sum_2 \bar{M}_c(2) + \bar{G} - \sum_2 G_c(2) \bar{M}_c(2), \quad (82)$$

where the bar denotes “approximate.” The expression (82) is highly implicit and incomplete until a rule is given for computing $G$ and $\bar{M}$. We now show how to choose $G$ and $\bar{M}$ in such a way as to achieve consistency.

Step (b): Take

$$\bar{G}_n[\bar{M}, v] = \bar{G}_n(1) = \frac{\delta \overline{\Phi}}{\delta \bar{M}_n(1)}, \quad (83)$$

which is still a functional of the unknown $\bar{M}$’s.

Step (c): Define $\bar{M}$’s as solutions of (42),

$$\bar{M}_n(1) = \left[ \exp \sum_{i=1}^n G_i(1) \frac{\delta}{\delta \bar{h}_i} \right] \bar{M}_n^0[1; \bar{h}_i = h(1)]. \quad (84)$$

This finally makes (82) and (83) explicit.
It is now easy to show by direct differentiation of (82) that
\[
\frac{\delta W}{\delta h}(1) = \mathcal{M}_1(1). \tag{85}
\]
In effect and for the approximate \(W\), this simply reverses the steps which lead from (51) to (60). To get the pair correlations, one need only take another field derivative of (85). It is advantageous to perform the calculation a little more generally. From (84)
\[
\frac{\delta \mathcal{M}_n(1)}{\delta h(2)} = \delta(12)\mathcal{M}_{n+1}(1) + \sum_{l,k} \mathcal{M}_{n+1}(1) I_{l,k}^{(13)} \frac{\delta \mathcal{M}_{l,k}(3)}{\delta h(2)}. \tag{86}
\]
Now, \(G\) depends on \(h\) only through the semi-invariants \(\mathcal{M}\), so, using the chain rule,
\[
\frac{\delta \mathcal{M}_n(1)}{\delta h(2)} = \delta(12)\mathcal{M}_{n+1}(1) + \sum_{l,k} \mathcal{M}_{n+1}(1) I_{l,k}^{(13)} \frac{\delta \mathcal{M}_{l,k}(3)}{\delta h(2)}, \tag{87}
\]
where \(I\) is the symmetric matrix,
\[
I_{l,k}^{(13)} = \frac{\delta^2 \Phi}{\delta \mathcal{M}_l^{(1)} \delta \mathcal{M}_k^{(3)}} \equiv \langle 1|l|3k\rangle. \tag{88}
\]
Finally, solution of (87) with \(n = 1\) gives,
\[
\mathcal{M}_2(12) = \sum_{l,k} \langle 1|l|3k\rangle \mathcal{M}_1(1) I_{l,k}^{(13)} \mathcal{M}_1(2). \tag{89}
\]
A few examples will serve to make the above more concrete:

1. The Effective-field Approximation
This well known approximation (Smart, 1966), the analog of the Hartree approximation in quantum statistics, follows from the choice at Step (a) of (see eqn (55)) \(\Phi[\mathcal{M}, v] = \frac{1}{2} \mathcal{M}_1(2)\) and corresponds to the sum of all bare free energy graphs (20) and Rule 1) having no closed loops. Physically the effective-field approximation is expected to be best for systems with long-range interactions, although it is worth emphasising that effective-field critical behaviour has no relation to reality for any physical system with finite range interactions.
Continuing to Step (b) we find,
\[
\mathcal{G}_1(1) = \sum_{l} v(12) \mathcal{M}_1(2) \quad \text{and} \quad \mathcal{G}_n = 0, \quad n > 1. \tag{90}
\]
Thus (Step (c)),
\[
\mathcal{M}_n(1) = \left[ \exp \mathcal{G}_1(1) \frac{\delta}{\delta h} \right] M_n(1; \beta) |_{H = H(1)} = M_n(1; \beta) \left[ \frac{\delta}{\delta h} \right] |_{H = H(1)} \tag{91}
\]
For \(n = 1\) and in the translationally invariant situation (21) this reduces for \(s = \frac{1}{2}\) to the well-known self-consistency condition,
\[
M_1 = \tanh (h + V(0)M_1), \tag{92}
\]
where \(V(0) = V(k = 0)\). The free energy in this approximation is
\[
\frac{W}{N} = \ln \left[ \exp (h + V(0)M_1) + \exp (-h - V(0)M_1) \right] - \frac{1}{2} V(0)M_1^2. \tag{93}
\]
Finally, from (88)
\[
I_{m}(12) = \frac{1}{2} v(12), \quad \text{when} \quad l = n = 1 \tag{94}
\]
and
\[
I_{m}(k) = \begin{cases} v(12), & \text{when} \ l = n = 1 \\ 0, & \text{otherwise} \end{cases} \tag{94}
\]
and
\[
\mathcal{M}_2(2) = \sum_{l} e^{-\Delta \tau} \mathcal{M}_1(2) = \frac{\mathcal{M}_2}{1 - \mathcal{M}_2 V(k)}. \tag{95}
\]

2. Ring graphs:
The first correction to the effective-field approximation in powers of the inverse range of the potential is usually taken to be the inclusion of \(\Phi\) of graphs with ring topologies.$^\dagger$ Here, therefore, we choose (Bloch and Langer, 1965; Horwitz and Callen, 1961),
\[
\Phi[\mathcal{M}, v] = \frac{1}{2} \mathcal{M}_1 + \frac{1}{2} \mathcal{M}_2 + \cdots + \frac{1}{2n} \left[ \mathcal{G}_n \right] \tag{96}
\]
with
\[
\mathcal{G}_1(1) = \sum_{l} v(12) \mathcal{M}_1(2), \tag{96}
\]
\[
\mathcal{G}_2(1) = \frac{1}{2} \left[ \mathcal{G}_1 + \mathcal{G}_1 \right], \tag{97}
\]
\[
\mathcal{G}_n = 0 \quad \text{for} \quad n > 2. \tag{97}
\]

$^\dagger$ The inverse-range expansion loses its meaning in the critical region and the above language is intended to be suggestive only (Horwitz and Callen, 1961; Englert, 1963).
$^\ddagger$ The quantum analog of the ring approximation is the self-consistent dielectric, bubble, or \(K\)-approximation. Propagator lines become points and correspond to our vertex functions.
In the translationally invariant limit,

$$\bar{G}_1 = V(0)\bar{M}_1, \quad \bar{G}_2 = \frac{1}{N} \sum_k e^{ikr} \frac{V(k)}{1 - \bar{M}_2 \bar{V}(k)},$$

so that the two fundamental semi-invariants are determined (Step (c)) by the non-linear coupled equations:

$$\bar{M}_1 = \left[ \exp \bar{G}_2 \frac{\partial^2}{\partial \bar{k}^2} \right] M_1 \bar{V}(\bar{k} + V(0)\bar{M}_1)|_{\bar{k}=0}$$

$$\bar{M}_2 = \left[ \exp \bar{G}_2 \frac{\partial^2}{\partial \bar{k}^2} \right] M_2 \bar{V}(\bar{k} + V(0)\bar{M}_1)|_{\bar{k}=0},$$

which can, for example, be recast along the lines of (50).

The matrix $I$ now has (in its valence indices) two non-vanishing components

$$I_{11}(12) = \sigma(12),$$

$$I_{22}(12) = \frac{1}{4}[C(12)]^2.$$  \hspace{1cm} (100)

I. Analysis of the two-point function

Before proceeding to the two-point or bond renormalisation, we must analyse the structure of the 2-rooted graphs and their contributions to the correlations $M_2$ more carefully than heretofore (De Dominicis, 1962; Stell, 1964).

Disassembly of a vertex pair

A vertex pair $V_1$ and $V_2$ of a (1-irreducible) graph $G$ is disassembled by the following procedure:

(i) Clip away all edges from both $V_1$ and $V_2$ (thereby dividing $G$ into a number of disjoint parts).

(ii) Reattach to $V_1$ and $V_2$ all clipped edges belonging to disconnected parts containing external vertices.

(iii) If there are any additional disconnected parts,

(a) rejoin the clipped ends of each ($V_1$ ends and $V_2$ ends separately)

(b) insert in the rooted part a single edge joining $V_1$ and $V_2$.

This process is pictured for several graphs in Fig. 10. The definitions which follow refer to 1-irreducible graphs.

Graphical definitions III

The unrooted parts formed in the process of disassembly are called 2-insertions. A 2-insertion which is not simply a bond is complex.

An articulation pair of a rooted graph is a pair of vertices the disassembly of which produces either one complex 2-insertion or any two or more 2-insertions. An articulation pair of an unrooted graph is a pair of vertices the disassembly of which produces either two complex 2-insertions or any three or more 2-insertions.

A graph is 2-irreducible if it contains no articulation pairs.

The 2-skeleton of a rooted graph is the graph produced by disassembling all pairs of vertices and discarding all 2-insertions thereby produced.

The following definitions classify important types of 2-rooted graphs:

The 2-rooted graph consisting of a single edge joining the external vertices is called the bond graph.

An internal vertex of a 2-rooted graph is said to be a nodal point if all paths between the two external vertices pass through it. A graph is nodal if it contains one or more nodal points; otherwise it is non-nodal.

Fig. 11. Various 1-irreducible 2-rooted graphs: (a) the bond graph; (b) a simple nodal graph (two nodal points); (c) a ladder graph; (d) a simple, nodal graph; (e) an elementary graph (contains one internal articulation pair); (f) the lowest order elementary graph.
A 2-rooted graph is simple if it is not the bond graph and if disassembly of its external vertices produces exactly one 2-insertion. A 2-rooted graph is a ladder graph if it is neither a bond graph nor a simple graph, i.e. if disassembly of its external vertices produces two or more 2-insertions.

A 2-rooted graph is elementary if it is both simple and non-nodal.

Examples of these definitions are given in Fig. 11.

Let us now consider the contributions of these various types of graph to the two-point cumulant correlations \( \mu_2(12) - \delta(12)M_2(1) \) (eqn (29) or (44)) or the related two-point parts of the higher correlations, e.g. (31). We use the vertex renormalised form of the expansions. It is convenient to sort the contributing graphs according to their valence at the external vertices and to supply by hand appropriate vertex factors at the external vertices. We therefore define as fundamental quantities the \( l, n \)-valent correlation factors,

\[
C_{ln}(12) = \begin{cases} \text{sum of all topologically distinct 1-irreducible} \\ \text{2-rooted connected graphs, which are} \\ \text{\( l \)-valent at} \\ \text{the external vertex 1 and} \\ \text{\( n \)-valent at the external} \\ \text{vertex 2, according to Rule 11.} \\ \end{cases}
\]  

(101)

**Rule 11: \( l, n \)-valent Correlation Factors \( C_{ln} \), Vertex Renormalised Form**

(a) Assign labels 1 and 2 to the external vertices and dummy labels to all internal vertices.

(b) For each edge joining vertices \( i \) and \( j \) write a factor \( v(ij) \).

(c) For each \( k \)-valent internal vertex \( i \) write a factor \( M_k(i) \). For each external vertex write a factor 1.

(d) Sum each internal vertex label freely over the entire lattice.

(e) Divide by the symmetry factor of the 2-rooted graph.

For example,

\[
C_{11}(12) = \frac{1}{2} \biggr( \begin{array}{c} 1 \biggr) + \biggr( \begin{array}{c} 1 \biggr) + \biggr( \begin{array}{c} 1 \biggr) + \biggr( \begin{array}{c} 1 \biggr) + \biggr( \begin{array}{c} 1 \biggr) + \biggr( \begin{array}{c} 1 \biggr) \biggr) + \text{order } v^5 \text{ and higher},
\]

(102)

The graphs contributing to (44) by Rule 5 may be classified according to valence at the external vertices, so (44) may be re-expressed, in terms of the correlation factors,

\[
\mu_2(12) = M_2(1)\delta(12) + \sum_{l,n=1}^{\infty} M_{l+1}(1)C_{ln}(12)M_{n+1}(2).
\]  

(103)

We now proceed to analyse \( C \) into its constituent graphical parts. The motivation for this analysis is that it will allow us to invert the relation (101) \( C[M,v] \) to provide \( v[M,C] \). This expression plays a role in the bond renormalisation of Section II.J equivalent to that of eqn (48) in the vertex renormalisation of Section II.E: \( C \) is determined as the solution of a complicated integral equation, thus buying enormous graphical simplification at the expense of increased algebraic complexity.

All contributions to \( C \) may now be classified according as they are nodal (\( N \)) or non-nodal (\( I \)),

\[
C_{ln} = I_{ln} + N_{ln},
\]  

(104)

where, for example,

\[
I_{11} = \quad \text{(exact)},
\]

\[
I_{21} = I_{12} = 0 \quad \text{(exact)},
\]

\[
I_{22}(12) = \frac{1}{2} \biggr( \begin{array}{c} 1 \biggr) + \biggr( \begin{array}{c} 1 \biggr) + \biggr( \begin{array}{c} 1 \biggr) + \biggr( \begin{array}{c} 1 \biggr) \biggr) + \text{order } v^5 \text{ and higher}. \quad (105)
\]

The non-nodal part \( I \) is derivable from the functional \( \Phi[M,v] \), eqn (54), Rule 7, (see also eqn (88)),

\[
I_{ln}(12) = \frac{\delta^2\Phi[M,v]}{\delta M_l(1)\delta M_n(2)},
\]  

(106)

so that (105) can be checked by direct differentiation of the first few terms of (55). The non-nodal property of \( I \) follows from the fact that \( \Phi \) is 1-irreducible. As in the expression (56) for \( G_n \), the essential point is that the presence of identical contributions from vertex pairs in \( \Phi \) which are topologically equivalent lowers the symmetry of the unrooted graph to that of the corresponding 2-rooted graph. Nodal contributions may be classified according to the number of nodal points:

\[
N_{ln}(12) = \sum_{3k,m} I_{ln}(13)M_{k+m}(3)I_{mn}(32)
\]

\[
+ \sum_{35,k,m,s} I_{ln}(13)M_{k+m}(3)I_{ms}(34)M_{s+n}(4)I_{sn}(42) + \ldots.
\]  

(107)
Again, the essential observation is that the symmetry factor of a nodal graph is just the product of the symmetry factors of its non-nodal components. A matrix notation is useful:

\[
\langle I | I | n \rangle_2 = I_{\text{in}}(12), \\
\langle I | M | n \rangle_2 = \delta(12)M_{1+n}(1), \\
\langle I | C | n \rangle_2 = C_{\text{in}}(12),
\]

(108)

where matrix multiplication involves a sum over valences and lattice points. It is easy formally to write \( C \) in terms of \( I \),

\[
C = I(1 - MI)^{-1},
\]

(109)
or inverting,

\[
I = (1 + CM)^{-1}C, \quad N = C - (1 + CM)^{-1}C,
\]

(110)

which will be useful below.

![Diagram](image.png)

*Fig. 12.* A ladder graph and its symmetry factor. The symmetry factor is composed multiplicatively of the symmetry factors of the simple or bond insertions \((2 \times 2 \times 1 \times 1 \times 1)\) and factorials due to the presence of identical insertions \((2! \times 3!)\).

The general 2-rooted graph is either a bond graph, a simple graph \((S)\), or a ladder graph \((L)\),

\[
C_{\text{in}} = v_{\text{in}} + S_{\text{in}} + L_{\text{in}},
\]

(111)

where

\[
v_{\text{in}}(12) = \begin{cases} v(12), & l = n = 1 \\ 0, & \text{otherwise.} \end{cases}
\]

(112)

Each ladder graph \( L \) is composed of two or more simple or bond graphs glued together at the external vertices (see e.g. Fig. 11(b) and (f)). The symmetry factor for the ladder graph is just the product of the symmetry factors for the individual insertions times a product of factorials due to the presence of identical 2-insertions, as illustrated in Fig. 12. Therefore, \( C \) can be written entirely in terms of \((v + S)\),

\[
C_{\text{in}} = (v + S)_{\text{in}} + \frac{1}{2} \sum_{k, m \neq l} \delta(l - k - m)(v + S)_{km}(v + S)_{lm} \delta(n - m - l) + \ldots,
\]

(113)
or in matrix notation,

\[
C = \left(e^{v+S} - 1\right),
\]

(114)

where the \( \delta \)-functions, which guarantee proper valence at the external vertices, have been left implicit. Equation (114) can, of course, be inverted to give \((v + S)\) in terms of \( C \). Substitution in (111) evaluates,

\[
L = C - \ln (1 + C),
\]

(115)
or, more explicitly expanding the logarithm,

\[
L_{\text{in}}(12) = \frac{1}{2} \sum_{k, m \neq l} \delta(l - k - m)C_{\text{in}}(12)C_{\text{in}}(12)\delta(n - m - t) \\
- \sum_{k, m \neq l} \delta(l - k - m - n)C_{\text{in}}(12)C_{\text{in}}(12)\delta(n - m - t - v) + \ldots
\]

(116)

Having succeeded in expressing \( L[C] \) and \( N[M, C] \), we now make the crucial observations that all non-nodal graphs are bond, ladder, or elementary,

\[
L_{\text{in}} = v_{\text{in}} + L_{\text{in}} + E_{\text{in}},
\]

(117)
or, alternatively, that all simple graphs are either nodal or elementary,

\[
S_{\text{in}} = N_{\text{in}} + E_{\text{in}}.
\]

(118)

When combined with (104) or (111), respectively, these give

\[
C_{\text{in}} = v_{\text{in}} + N_{\text{in}} + L_{\text{in}} + E_{\text{in}}.
\]

(119)

Now, solve for \( v \) and substitute (110) and (115),

\[
v = (1 + CM)^{-1}C - C + \ln (1 + C) - E.
\]

(120)

This constitutes \( E[M, C] \) provided we can express \( E[M, C] \), which will be done in Section II.J. The lowest order elementary graph is shown as Fig. 11(f).

The approximation \( E = 0 \) in (120) provides an integral equation for \( C \), which in the context of the classical fluid is called the hypernetted chain equation (Van Leuven et al., 1959; Meeron, 1960; Stell, 1964). The corresponding equation in the magnetic case was first derived by Englert (1963) and has been studied by Orlans (1963).

**J. Renormalisation of the interaction**

Bond or interaction renormalisation is the name given to the next (two-point) level of selective resummation. The development is closely parallel to Section II.E. There \( M^0 \) was replaced by \( M \) as the graphical vertex element with a consequent restriction to 1-irreducible graphs. Here we will replace the potential \( v \) by the general two-point correlation factor \( C \) introduced in (101).

Consider a general 1-irreducible \( n \)-rooted connected graph, \( n \geq 3 \). Such a graph has a unique 2-irreducible 2-skeleton defined (in Section II.I) by
successive disassembly of all vertex pairs, a process which for each pair of vertices cuts away all 2-insertions and replaces them by a single edge. Conversely, every such graph can be constructed in a unique way by decorating its underlying 2-skeleton, i.e., replacing each edge in turn by an appropriate 1-irreducible 2-rooted graph. This process is illustrated in Figure 13. It produces every 1-irreducible n-rooted graph once and only once.

Fig. 13. A 3-rooted graph reduced to (built up from) its 2-skeleton.

Summation of all graphs having the same 2-skeleton is now accomplished simply by reinterpreting skeletal lines as the correlation factor $C$ (instead of $v$). As in the case of vertex renormalization, the only subtle point is that the symmetry factors work out. In building each 1-irreducible (but not 2-irreducible) graph by decoration of its 2-skeleton, the symmetry factor of each 2-rooted decoration enters multiplicatively. The lowering of skeletal symmetry due to distinct decorations of previously equivalent skeletal edges is taken care of by the cross-terms in the product of $C$’s for the bond-renormalised graph.

We illustrate by treating the 3-point correlations $M^s_3$, eqn (31), explicitly. Note first that the two-point parts $M^s_{21}(12)$, etc., may, by a trivial extension of the reasoning leading to (103), be written as,

$$ M^s_{21}(12) = \sum_{l=1}^{n} l^1_{12} l^2_{12} M_{l_1 l_2}(12) M_{l_1 l_2}(2). \tag{121} $$

The full expression then is,

$$ M^s_{3}(123) = \delta(123) M^s_{3}(1) - \delta(12) M^s_{21}(13) - \delta(13) M^s_{21}(32) - \delta(23) M^s_{21}(21) 
= \text{sum of all topologically distinct 3-rooted 2-irreducible connected graphs according to Rule 12.} \tag{122} $$

Rule 12: Three-point Correlations, Vertex and Bond Renormalised Form

(a) Assign labels 1, 2, 3 to the external vertices and dummy labels to all internal vertices.

(b) For each edge joining vertices $i$ and $j$ write a factor $C_{i,j}(ij)$.

† There is a close parallel here with the discussion surrounding eqn (43), particularly if one chooses (as we shall not) to discuss the decoration in terms of constituent 2-insertions.

To write the proper vertex factors it is convenient to define the generalised valence ($g$-valence) $n_i$ of a vertex $i$ as,

$$ n_i = \sum_{\text{incident edges}} l_i, $$

i.e., the $g$-valence is obtained by summing the valence labels $l_i$ of all correlation factors incident at $i$.

(c) For each internal vertex $i$ of $g$-valence $n_i$ write a factor $M_n(i)$. For each external vertex $i$ of $g$-valence $n_i$ write a factor $M_{n+1}(i)$.

(d) Sum each internal vertex label freely over the entire lattice. Sum all valence labels $l_i = 1, 2, \ldots$

(e) Divide by the symmetry factor of the 3-rooted graph.

The first few graphs in the sum (122) are,

$$ + \text{order } C^4 \text{ and higher.} \tag{123} $$

As an application of Rule 12, the fifth term in (123) is,

$$ \sum_{i,j,k} C_{i,j,k}(14) C_{i,j,k}(24) C_{i,j,k}(34) M_{l_1+1, l_2+1, l_3+1}(4) M_{l_1, l_2+1}(2) M_{l_1+1, l_2, l_3, l_4}(3). \tag{124} $$

Formulations such as (122) are only useful if correlation factors $C$ are known, so we must return to the problem raised in Section II of finding the relation $E[M, v]$ whose inversion $C[M, v]$ evaluates the correlations. Expression (120) lacks only $E[M, v]$. All elementary 2-rooted graphs may be obtained by decoration of 2-rooted graphs which are elementary and contain no articulation pair except the pair consisting of the two external vertices.† Such graphs will be called elementary 2-rooted 2-skeletons.

To express $E_{\mu
u}$ then, one calculates the contributions of all $l, n$-valent elementary 2-rooted 2-skeletons according to Rule 13.

Rule 13: Elementary Correlation Factors, Vertex and Bond Renormalised Form

(a) Assign the labels 1 and 2 to the external vertices and dummy labels to all internal vertices.

† The two external vertices of a 2-rooted graph are always an articulation pair. Disassembly at the external vertices leaves the bond graph.
(b) For each edge joining vertices \(i\) and \(j\) write a factor \(C_{ij}(ij)\).

(c) For each internal vertex \(i\) of \(g\)-valence \(n_i\) (see Rule 12) write a factor \(M_{n_i}(i)\). For each external vertex write a factor 1.

(d) Sum each internal vertex label freely over the entire lattice. Sum all valence labels \(l_i = 1, 2, \ldots\).

(e) Divide by the symmetry factor of the 2-rooted graph.

The first few terms are:

\[ E_{11}(12) = \frac{1}{2} + \frac{1}{2} + \frac{1}{2} + \frac{1}{2} + \frac{1}{2} + \frac{1}{2} + \frac{1}{2} + \text{graphs with at least four internal vertices}. \] (125)

There are 56 distinct elementary 2-rooted 2-skeletons with four internal points, not counting as distinct graphs which differ only through interchange of external vertices (such as the third and fourth or seventh and eighth graphs in (125)).

\[ \frac{1}{2} = \frac{1! \cdot 2!}{3!} \left[ \frac{1}{2} + \frac{1}{2} + \frac{1}{2} + \frac{1}{2} \right] \]

Fig. 14. A self-field graph (1-insertion) can be formed by superposing the external vertices of the corresponding 2-rooted simple graphs. See eqn (126).

The self-fields \(G_{s}\) may be expressed in terms of the correlation factors \(C_{tr}\). The general relation is,

\[ G_{l+n}(1) = \frac{l! n!}{(l+n)!} S_{n}(11). \] (126)

The presence only of simple graphs on the right of (126) guarantees that the result of superposing root points will be a 1-insertion. The factorials compensate for the difference in symmetry factors between the 1-rooted and 2-rooted graphs and the fact that a given 1-insertion may be obtained from several distinct simple graphs, as illustrated in Fig. 14. Equation (126) can be expressed directly in terms of \(C\) by using (114) and noting \(v(11) = 0\),

\[ G_{l+n}(1) = \frac{l! n!}{(l+n)!} \langle l!|l|n|C|n1\rangle. \] (127)

The full renormalisation \([M^0, v] \rightarrow [M, C]\) is then expressed by equation (48) and (120),

\[ M^0 = e^{-\beta C} M, \]

which inverts the bare perturbation-theoretic relations \(M[M^0, v]\) (28) and \(C[M^0, v]\). The only graphical part of (128) is \(E[M, C]\), eqn (125), which (although it is still an infinite graphical sum) requires enormously fewer graphs to any given order in \(v\) than analogous bare expansions such as (30).

On the other hand, regarded as an integral equation for \(C\) in terms of \(v\), eqn (128) is highly non-linear. Even the simplest approximation \(E = 0\) (Orlińska, 1963) cannot be solved exactly.

Iterative solution in powers of \(v\) (Ferer et al., 1969; Moore et al., 1969) is simple in principle though still time-consuming. To find all terms in \(M\) and \(C\) up to a given power of \(v\), one needs only a finite number of graphs in \(E\). In zero field, for example, \(E\) first enters in order \(v^7\) and the single graph Fig. 11(f) suffices through order \(v^8\) (\(v^9\) with nearest-neighbour interactions only on loose-packed lattices). It is convenient to iterate simultaneously both of eqns (128). Once the \(M\)'s and \(C\)'s are known from (128) or some approximation thereto, then (103) gives the pair correlations \( MH(12)\) and (122) (and higher order analogues) give \( M\) for \(n > 2\).

To complete the story we need an expression for \(W[M, C]\), the fully renormalised generalisation of the vertex renormalised (60). This derivation can be done topologically in analogy to De Dominicis' work on the classical fluid (De Dominicis, 1962). The algebraic derivation (Wortis et al., 1969) simply integrates eqn (7). To carry out this integration efficiently it is necessary to introduce a slight generalisation of our present development. We merely quote the result (Wortis et al., 1969),

\[ W = \sum_{l} M_{0}(1) - \sum_{l} \sum_{l_1} G_{l}(1) M_{l}(1) + \frac{1}{2} \sum_{l_1, l_2} v(12) \left[ MH(12) + MH(1)MH(2) \right] + \Omega[M, C], \] (129)

where

\[ \Omega[M, C] = \frac{1}{2} \sum_{l_1, l_2, l_3} M_{l}(1) \langle l|l||C - (1 + C) \ln (1 + C)|2n\rangle M_{l}(2) \]

\[ + \frac{1}{2} \text{Tr}[\ln (1 + MC) - MC + \frac{1}{2} \text{MCMCM}] \]

\[ + \{\text{sum of all topologically distinct 2-irreducible unrooted graphs} \} \]

†The graphs \(\bullet\), \(\circ\), and \(\diamond\) are specifically excluded.
Rule 14: The Functional $\Omega[M, C]$, Vertex and Bond Renormalised Form

(a) Assign dummy labels to all internal vertices.
(b) For each edge joining vertices $i$ and $j$ write a factor $C_{i,j}(ij)$.
(c) For each internal vertex of $g$-valence $n_i$ (see Rule 12) write a factor $M_{n_i}(i)$.
(d) Sum each internal vertex label freely over the entire lattice. Sum all valence labels $l_i = 1, 2, \ldots$
(e) Divide by the symmetry factor of the unrooted graph.

The trace in (130) refers to the matrix representation (108), e.g.

$$\frac{1}{4!} \text{Tr} [\ln (1 + MC)] = \frac{1}{4!} \sum_{n=1}^{\infty} \sum_{n=1}^{\infty} \langle n_1 | \ln (1 + MC) | n_1 \rangle. \quad (131)$$

The first four terms in the graphical sum are,

$$\frac{1}{4!} \quad + \quad \frac{1}{12} \quad + \quad \frac{1}{5!} \quad + \quad \text{graphs with six or more vertices.} \quad (132)$$

The evaluation (130) is, of course, not necessary in series calculations, since, once $\mathcal{M}_1$ and $\mathcal{M}_2$ are known explicitly to a given order in $v$, eqn (7) can be integrated term-by-term.

K. Further renormalisation: comments

Vertex (1-point) and interaction (2-point) renormalisations have now been carried out explicitly. De Dominicis (1962) has given a very brief discussion of 3-point renormalisation for the classical fluid. We shall not develop higher order renormalisations, but the lines which such a development would follow should now be apparent: l-vertex disassembly defines l-insertions and an l-skeleton. All order $n$ correlations $n > l$ can be summed by decorating l-skeletons with combinations of l-insertions. The only point requiring finesse is the derivation of the higher order analogs of eqns (128), expressing the l-order potentials (identically zero for the Ising model) in terms of the l-correlation factors.

III. Further Applications and Extensions of the Linked-Cluster Expansion

A. Orientation

The linked-cluster expansion was developed in detail in Section II for the specific example of the spin $s$ Ising model. This is the simplest and most studied application. The bare graphical expansions of Section II.B were renormalised with respect to vertices in Sections II.E and II.F and then with respect to edges in Sections II.I and II.J. The renormalisation process depended on two quite general properties, (i) graph topology and (ii) the freedom of the lattice sums in part (d) of all graphical rules.

Linked-cluster expansions closely analogous to the Ising expansion exist for a wide variety of other systems, both quantum and classical. The criterion is simply that the system be spatially local in the absence of interactions. Once a bare (unrenormalised) expansion is known to exist which is graphical and contains free lattice sums, its renormalisation is immediate. The presence of extra variables, non-commutativity of operators, etc., present only clerical problems and have no influence on the arguments leading to renormalisation.

In this section we shall briefly sketch some of these extensions and generalisations. Our purpose will be to reduce the analysis to a stage where the Ising development is clearly applicable. Generalisation of results from Section II can then be written down by inspection. The subsections which follow are intended to be independent of one another, although they will draw extensively on the material of Section II.

B. Inclusion of additional local fields

Inclusion in the Hamiltonian (1) or (2) of additional spatially local fields is a useful if trivial generalisation. Consider, for example, the dimensionless Hamiltonian,

$$- \beta \mathcal{H} = \frac{1}{2} \sum_{i,j} \sigma(12) \mu(1) \mu(2) + \sum_i h(i) \mu(1) + \sum_i \sigma(1) X(1), \quad (133)$$

where $X(1)$ is a local operator belonging to the dynamical subsystem at site 1 and $\sigma$ is an external field which couples locally to $X$. For example, a single-ion magnetic anisotropy would be written with $X(1) = \mu^2(1)$ and $\sigma(1)$ the local anisotropy field.$^\dagger$

The free energy $W$ is now a functional of $\sigma$ in addition to $h$ and $v$, $W[h, \sigma, v]$. The Ising derivative relations (4)–(8) continue to hold; however, in addition,

$$\frac{\delta W}{\delta \sigma(1)} = \langle X(1) \rangle, \quad \frac{\delta^2 W}{\delta \sigma(1) \delta \sigma(2)} = \langle X(1) X(2) \rangle - \langle X(1) \rangle \langle X(2) \rangle, \text{etc.} \quad (134)$$

$^\dagger$ This model, which has been studied for $s = 1$ by Griffiths (1970), Blume et al. (1971), and Oitmaa (1970), is interesting in that (at least in the effective-field approximation) it exhibits either a second order transition, a first order transition, or no transition at all depending on the value of $\sigma$. No
The initial condition (9) and (10) is modified by $\Delta$,

$$W_0[h, \Delta] = \sum_i M_0^0(1) = \sum_i \left[ \ln \sum_{\mu = -1}^{+1} \exp \left[ h(1) \mu + A(1) X \right] \right].$$  \hfill (135)

For example, in the Griffiths–Blume model referred to above,

$$M_0^0(1) = M_0^0(1; h, \Delta) = \ln (1 + 2 e^h \cosh h).$$  \hfill (136)

The bare semi-invariants continue to be defined by (14),

$$M_n^0(h, \Delta) = \frac{\partial^n}{\partial h^n} M_0^0(h, \Delta),$$  \hfill (137)

but now depend parametrically on $\Delta$ at each site.

In the development of unrenormalised perturbation theory, the semi-invariants appeared as derivatives of $W_0$, i.e. directly in the form (137). Thus, Rules I through 4 (eqns (20), (28), (30), and (31)) are unchanged except that they are now to be carried out in terms of the bare semi-invariants (135), (137), instead of (10), (14). The subsequent renormalisation, which simply replaces the bare semi-invariants $M_n^0$ by their renormalised analogs, goes through unchanged.

Once having incorporated $\Delta$ as a parameter into the semi-invariants, it is extremely easy to generate correlations involving the operators $X$. The procedure mimics the discussion preceding eqns (27)–(31). For example, to find $\langle X \rangle$ using (14), we note that $\Delta$ appears in the unrenormalised expansion for $W$ only through the semi-invariants, so, schematically,

$$\delta W \delta \Delta(1) = \sum_{n=0} \delta W[M_0^0, v] \frac{\partial M_n^0(1)}{\partial \Delta(1)}.$$  \hfill (138)

In graphical terms, $\delta W/\delta M_0^0$ roots one $l$-valent vertex of a previously un-rooted graph and $\delta M_0^0(1)/\delta \Delta(1)$ replaces the semi-invariant at that vertex by a new type of mixed semi-invariant generated from $M_0^0(h, \Delta)$ by both $h$ and $\Delta$ derivatives. Denote

$$M_{l,n}^0(h, \Delta) = \frac{\partial^l}{\partial h^l} \frac{\partial^n}{\partial \Delta^n} M_0^0(h, \Delta).$$  \hfill (139)

Then (cf. (28)),

$$\langle X(1) \rangle = \left\{ \begin{array}{c}
\text{sum of all topologically distinct} \\
\text{1-rooted connected graphs according} \\
to \text{Rule 2'}. \end{array} \right\}$$  \hfill (140)

Rule 2':

Same as Rule 2 for $n = 1$ except:

(c) For each $l$-valent internal vertex $i$ write a factor $M_i^0(i)$. For each $l$-valent external vertex write a factor $M_{l,1}^0(1)$.

Since the operator $X$ is not coupled to the interaction, it appears only at external vertices, and the generalised semi-invariants (139) $n \neq 0$ do not enter self-fields. Thus, vertex renormalisation of the generalised semi-invariants follows (42),

$$M_{l,n}(1) = \left[ \exp \sum_{k=1}^{\infty} G[k; M, v] \frac{\delta^k}{\delta \Delta^k} \right] M_{l,n}^0(1; h, \Delta) \Delta^{k(1)}.$$  \hfill (141)

The analog of (45) is

$$\langle X(1) X(2) \rangle = \langle X(1) \rangle \langle X(2) \rangle + \left\{ \begin{array}{c}
\text{sum of all topologically distinct} \\
2\text{-rooted 1-irreducible connected} \\
\text{graphs according to Rule 5'}. \end{array} \right\}$$  \hfill (142)

Rule 5':

Same as Rule 5 except:

(c) For each $l$-valent internal vertex $i$ write a factor $M_i(i)$. For each $l$-valent external vertex $i$ write a factor $M_{l,1}(i)$.

Correspondingly, the analogue of (103) is,

$$\langle X(1) X(2) \rangle = \delta(12) M_{0,2}(1) + \sum_{l,n=1}^{\infty} M_{l,1}(1) C_{l,n}(12) M_{n,2}(2),$$  \hfill (143)

so that, if the correlation factors $C$ have been found in the calculation of $M_{2}(12)$, the extra work required to complete the $X-X$ correlations is minimal.

C. Several commuting variables: the classical Heisenberg model

The first application of the linked-cluster method to the derivation of the high-temperature expansions useful in the study of critical phenomena was in connection with the anisotropic classical Heisenberg model. Joyce (1967) developed the unrenormalised form of the expansion by generalising the work of Horwitz and Callen (1961) and generated the first few terms in perturbation theory. Jasnow and Wortis (1968) and Jasnow (1969) applied the vertex renormalisation to go to higher orders. The Hamiltonian is,

$$H = - \sum_{a=\alpha, \beta, \gamma} J^a(i) a_i a_j - m \sum_i B(i) t_i,$$  \hfill (144)
where the sum is over distinct pairs \( i \neq j \), \( J(ij) \) is the exchange coupling between sites \( i \) and \( j \), \( m \) is the magnetic moment, and \( H(i) \) is the magnetic field at site \( i \). \( t \) is a classical unit vector associated with site \( i \). Rewriting (144) in dimensionless units,

\[
-\beta \mathcal{H} = \frac{1}{2} \sum_{i,j} v^s(2) t_i^s(1) t_j(2) + \sum_{s} \delta^s(1) \delta^s(1),
\]

where \( v = \beta J, h = \beta m H \), and numerical arguments stand for lattice sites. We define as usual,

\[
W[h, v] = \ln \text{Tr} \exp(-\beta \mathcal{H}),
\]

where the trace indicates integration of each unit vector \( t \) over its unit sphere. Cumulant correlations are generated via the second term on the right of (145),

\[
\frac{\delta^2 W}{\delta h^s(1) \delta h^s(2)} = \langle t_i^s(1) t_j^s(2) \rangle - \langle t_i^s(1) \rangle \langle t_j^s(2) \rangle = \mathcal{M}_{s}(12),
\]

and so forth, where the Greek subscripts stand for Cartesian coordinates and are paired with the space indices.

The differential equation which (in analogy to (8)) generates the linked-cluster expansion is

\[
\frac{\delta W}{\delta v^s(12)} = \frac{\delta^2 W}{\delta h^s(1) \delta h^s(2)} + \frac{\delta W}{\delta h^s(1)} \frac{\delta W}{\delta h^s(2)}. \tag{148}
\]

The non-interacting free energy \( W_0 \) is

\[
W_0[h] = \sum_{\gamma} M_0^0(1),
\]

\[
M_0^0(1) = M_0^0[1; h(1)] = \ln \int d\Omega \exp [h(1) \cdot t] \ln \left[ \frac{4\pi \sinh|h(1)|}{|h(1)|} \right]. \tag{149}
\]

The bare semi-invariants, which enter the Taylor series coefficients as the cumulant correlations associated with an isolated site, now carry an extra set of Cartesian subscripts,

\[
M_0^0(1, x_1 \ldots x_n) = \frac{\delta^2 M_0^0(1)}{\delta h^x(1) \ldots \delta h^x(1)},
\]

which is totally symmetrical in the \( x \)'s.

In constructing the Taylor development of the free energy \( W \) along the lines of (11), there is an extra Cartesian index \( x \) which goes with each potential factor \( v^x(12) \) and must be summed \( \forall x = x, y, z \). The two \( (\delta \delta h^x) \)'s which go with \( v^x \) by (148) tie each edge \( v^x \) to bare semi-invariants containing \( x \) at its two ends. The topology of the graphs on the other hand depends only on spatial structure and goes through exactly as for the Ising model. The rule for the unrenormalised free energy, which could also be derived along the lines of Section II.C, is (cf. Rule 1, eqn (20)),

\[
W[h, v] = \left\{ \begin{array}{l}
\text{sum of all topologically distinct unrooted} \\
\text{connected graphs according to Rule 15.}
\end{array} \right.
\]

**Rule 15: Classical Heisenberg Model Free Energy \( W \), Unrenormalised Form**

(a) Assign a dummy label to each internal vertex and a Cartesian index to each edge.

(b) For each edge indexed \( \gamma \) and joining vertices \( i \) and \( j \) write a factor \( v^\gamma(ij) \).

(c) For each \( I \)-valent vertex \( i \) write a factor \( M_0^0(i, \gamma_1 \ldots \gamma_I) \), where \( \gamma_1 \ldots \gamma_I \) are the Cartesian indices of the edges incident at \( i \).

(d) Sum each internal vertex label freely over the entire lattice. Sum the Cartesian index of each edge \( \gamma = x, y, z \).

(e) Divide by the symmetry factor of the unrooted graph.

Since topology is unchanged from the Ising case, the first few contributing graphs are given by (20). For example,

\[
\frac{1}{2} \mathcal{M}_s(12) = \frac{1}{2} \sum_{\gamma_1 \gamma_2} \sum_{\gamma_1 \gamma_2} v^{\gamma_1}(12) v^{\gamma_2}(23) M_0^0(1, \gamma_1) M_0^0(2, \gamma_1 \gamma_2) M_0^0(3, \gamma_2). \tag{151}
\]

Linked-cluster rules for the cumulant correlations are derived via (147). \( W[M^x, v] \) depends on the fields \( h \) only through the semi-invariants \( M^x \). Differentiation fixes a vertex, increases its order by one, and attaches a Cartesian label. The reduction of the unrooted symmetry factor to that appropriate to the rooted graph depends on topology alone and does not differ from the Ising case. As an example, we give the expression for the pair correlations (cf. Rule 3, eqn (30)), which are the easiest route to the susceptibility matrix:

\[
\mathcal{M}_{s}(12) - \delta(12) M_2^0(1, 2\beta) = \left\{ \begin{array}{l}
\text{sum of all topologically distinct} \\
\text{2-rooted connected graphs according} \\
\text{to Rule 16.}
\end{array} \right. \tag{152}
\]

\( \dagger \) For an interacting system of classical plane rotors (Bowers and Joyce, 1967; Stanley, 1968), the unit vector \( t \) is restricted to a plane. The trace operation is an angular integral from 0 to \( 2\pi \), thus changing the evaluation (149)-(150) of the semi-invariants. The sum over \( x \) is only \( x = x, y \). Otherwise, everything is exactly as here sketched.
Rule 16: Classical Heisenberg Model Pair Correlations, Unrenormalised Form

(a) Assign a dummy label to each internal vertex and a Cartesian index \( \gamma \) to each edge. Assign the pair \((x, 1)\) to one of the two external vertices and \((\beta, 2)\) to the other.

(b) For each edge indexed \( \gamma \) and joining vertices \( i \) and \( j \) write a factor \( v^\gamma(ij) \).

(c) For each \( l \)-valent internal vertex \( i \) write a factor \( M_0^\gamma(i, \gamma_1 \ldots \gamma_l) \). For each \( l \)-valent external vertex \( i = 1, 2 \) write a factor \( M_{l+1}^\gamma(i, \gamma_1 \ldots \gamma_l) \) with \( \gamma = x(\beta) \) for vertex \( 1(2) \). The indices \( \gamma_1 \ldots \gamma_l \) are the Cartesian labels of incident edges.

(d) Sum each internal vertex label freely over the entire lattice. Sum the Cartesian index of each edge \( \gamma = x, y, z \).

(e) Divide by the symmetry factor of the 2-rooted graph.

Contributing graphs are given by (30).

Renormalisations go through exactly as for the Ising model. The extra complexity introduced by the Cartesian sums is entirely clerical. The renormalisation of the semi-invariants will serve to illustrate this point. The self-field \( G_n(1) \) at the point 1 must now carry the \( n \) Cartesian indices of the edges incident at the external vertex. In the process of decoration, by which the renormalised semi-invariant is formed, each of these edges must be matched to the bare semi-invariant. Thus, the self-field (cf. Rule 6, eqn (47)),

\[
G_n(1, x_1 \ldots x_n) = \sum_{n \text{-valent at the external vertex}} \text{all topologically distinct } l \text{-irreducible } l \text{-insertions which are according to Rule 17.}
\]

(153)

Rule 17: Classical Heisenberg Model Self-Field, Vertex Renormalised Form

(a) Assign the Cartesian indices \( x_1, \ldots, x_n \) to the \( n \) edges incident at the external vertex 1. Assign a Cartesian index \( \gamma \) to each additional edge. Assign a dummy label to each internal vertex.

(b) For each edge indexed \( \gamma \) and joining vertices \( i \) and \( j \) write a factor \( v^\gamma(ij) \).

(c) For each \( l \)-valent internal vertex \( i \) write a factor \( M_0^\gamma(i, \gamma_1 \ldots \gamma_l) \) (the renormalised semi-invariant to be defined below). For the external vertex write a factor of 1.

(d) Sum each internal vertex label freely over the entire lattice. Sum the Cartesian indices of all edges not incident at the external vertex \( \gamma = x, y, z \).

(e) Divide by the symmetry factor of the 1-rooted graph.

Contributing graphs and symmetry factors are as given by eqn (47). One representative term in the evaluation of \( G_3 \) is shown in Fig. 15. Unlike the semi-invariants, \( G_n(1, x_1 \ldots x_n) \) is not in general symmetric under permutations of its Cartesian indices,† though it will, of course, reflect any symmetries of the Hamiltonian (144), (145). The renormalised semi-invariant is (cf. (42)),

\[
M_n(1, x_1 \ldots x_n) = \left[ \exp \sum_{l=1}^{\infty} \sum_{x_{\gamma_1}, \ldots, x_{\gamma_l}} G_l(1, x_1 \ldots x_n) \frac{\delta^l}{\delta h^{\gamma_1} \ldots \delta h^{\gamma_l}} \right] M_n^{0}(1, x_1 \ldots x_n; \hbar) |_{\hbar = \hbar(1)}. \tag{154}
\]

The vertex renormalised form of (152) sums \( l \)-irreducible 2-rooted graphs by a rule identical to Rule 16 except for the replacement \( M^0 \rightarrow M \).

\[
\frac{1}{2} \sum_{x, y, z} M_2^0(2, x_1 y) M_3^0(\gamma, z, x_2 y) \times M_2^0(2, x_1 y) M_3^0(3, x_2 z y).
\]

Fig. 15. A contribution to \( G_3 \).

Like \( G \), the correlation factors \( C \) must now carry Cartesian indices labelling lines at external vertices. Thus,

\[
M_{ap}(12) - \delta(12) M_2^0(1, \alpha \beta) = \sum_{\gamma=1}^{\infty} \sum_{\beta_1 \ldots \beta_n} M_{l+1}^\gamma(1, x_1 \ldots x_n) C_{\gamma \beta}(1, x_1 \ldots x_l; 2, \beta_1 \ldots \beta_2, n+1(2, \beta_2 \ldots \beta_n)).
\]

(155)

D. Non-commuting variables: the quantum Heisenberg model

In treating the quantum many-particle problem (Martin and Schwinger, 1959; Kadanoff and Baym, 1962; Abrikosov et al., 1965), it is customary to focus attention not on the operator \( \exp (-\beta \mathcal{H}) \), whose trace gives the thermodynamics, but rather on the time-ordered unitary operator,

\[
U(t_1, t_2) = \left[ \exp \left( -i \int_{t_1}^{t_2} dt \mathcal{H}(t) \right) \right]_+ \tag{156}
\]

which generates the time translations of the state vector of the system from time \( t_2 \) to time \( t_1 \). Time-dependence is therefore introduced \textit{ab initio} into the

† In the renormalisation, \( G \) is contracted with the symmetrical semi-invariant, thus picking out its symmetrical part, so it is possible to define \( G \) to be symmetrised without changing what follows.
formalism, making all calculation significantly more involved than is the case classically. This time-dependence also seems inescapable when dealing with magnetic systems, and it appreciably enhances the difficulty of practical algebraic calculation. However, it is important to emphasise at the outset that, once all definitions have been properly generalised, the topological properties of the theory are identical to those of the Ising model, discussed in Section II.

The Hamiltonian of the spin $s$ anisotropic Heisenberg Model is
\begin{equation}
\mathcal{H} = -\frac{1}{s^2} \sum_{\sigma \in \{1, \ldots, s\}} J^\sigma(i) s_{\sigma i} s_{\sigma j} + m \sum_i H(i) \cdot s_i.
\end{equation}
(157)

It is convenient to introduce the normalised operators $t(1) = [s(r_1, t_1) / s]$, where in dealing with quantum systems the numerical label 1 refers to both the lattice site $r_1$ and the time $t_1$. In units such that $\hbar = 1$, $t(1) \cdot t(1) = \left(1 + \frac{1}{s}\right)$, $t(1) \times t(2)|_{t_1 = t_2} = is\delta(r_1, r_2) \frac{t(1)}{s}$. (158)

In terms of the variables $J \equiv v, mH \equiv h$, then,
\begin{equation}
-\mathcal{H}(t) = \frac{1}{s^2} \sum_{r_1, r_2} \sum_{\sigma \in \{1, \ldots, s\}} u^\sigma(r_1, r_2) t_\sigma(r_1, t) t_\sigma(r_2, t) + \sum_{r_1, r_2} h^\sigma(r_1, t) t_\sigma(r_1, t).
\end{equation}
(159)

It is important in the development which follows formally to maintain $h$ and $v$ as functions of time independently variable for each point and bond.

Now, in the physical limit, in which $\mathcal{H}$ is time-independent, $U(t_1, t_2) = \exp(-i\mathcal{H}t) - U(-i\beta, 0) = \exp(-\beta\mathcal{H})$. This observation motivates the restriction of all time variables to the pure imaginary interval $[0, -i\beta]$, where for purposes of time-ordering “larger” times are those lying nearer $-i\beta$. Note that for a finite system with a bounded Hamiltonian (like (159)) there is certainly no difficulty in analytically continuing the generalised variables in (156). We shall not attempt to discuss the more formidable problem of the $N \to \infty$ limit. The proper definition of the generalised free energy $W$ in the presence of time-variation is
\begin{equation}
W[h, v] = \ln \text{Tr} U(-i\beta, 0).
\end{equation}
(160)

Functional differentiation† generates time-ordered correlation functions in
\begin{equation}
\mathcal{W}[h, v] = \langle t_\alpha(1) \rangle = \mathcal{M}_\alpha(1),
\end{equation}
(159)
which are restricted to $[0, -i\beta]$, 
\begin{equation}
(-i) \frac{\delta W[h, v]}{\delta h^\sigma(1)} = \langle t_\alpha(1) \rangle = \mathcal{M}_\alpha(1),
\end{equation}
(159)
\begin{equation}
(-i) \frac{\delta^2 W[h, v]}{\delta h^\sigma(1) \delta h^\rho(2)} = \langle (t_\alpha(1) t_\beta(2))_+ \rangle - \langle t_\alpha(1) \rangle \langle t_\beta(2) \rangle = \mathcal{M}_{\alpha\beta}(2).
\end{equation}
(161)

which should be compared with (147). In (161) all operators have Heisenberg time-dependence $X(t) = U^{-1}(t, 0)X(0)U(t, 0)$ and the expectation value is defined with respect to $U(-i\beta, 0)$,
\begin{equation}
\langle X \rangle = \frac{\text{Tr} U(-i\beta, 0) X}{\text{Tr} U(-i\beta, 0)}.
\end{equation}
(162)

The notation $(\cdot)_+$ indicates an ordering of all operators right to left by increasing times. The physical correlation functions (for real times) may be obtained from (161) and higher order analogs by analytic continuation in the time variables. Of course, $W$ requires no analytic continuation and, when $h$ and $v$ are time-independent, $\mathcal{M}_\alpha(1)$ is, too. The procedure for continuation is discussed at length in the many-particle literature and is not of immediate relevance to our present concerns, which are mainly topological. The analog of the functional differential equation (8) is
\begin{equation}
(-i) \frac{\delta W}{\delta \sigma^\rho(1)} = \langle t_\alpha(1) t_\beta(2) \rangle|_{t_1 = t_2}.
\end{equation}
(163)

In the absence of interaction (cf. (9) and (10)),
\begin{equation}
W[h, v = 0] = W_0[h] = \sum_\alpha M_\alpha O^{\alpha}(1),
\end{equation}
where
\begin{equation}
W_0 O^{\alpha}(1) = \ln \text{Tr} \left( \exp \int_0^{i\beta} \text{d} \tau \sum_\sigma h^{\sigma}(\tau) t_\sigma(\tau) \right)_+.
\end{equation}
(164)

The unrenormalised semi-invariants are now time-dependent,
\begin{equation}
M_\alpha^{\rho}(r, \tau_1 \ldots \tau_n) = \frac{(-i)^n \delta^{n} M_\alpha^{\rho}(r)}{\delta h^{\sigma_1}(r, \tau_1) \ldots \delta h^{\sigma_n}(r, \tau_n)}.
\end{equation}
(165)

Unlike (10) or (149), (164) cannot in general (i.e. for time-dependent $h$) be evaluated in closed form, so (165) cannot be used in a practical way to
evaluate the semi-invariants. This need not cause difficulty in practice, since \( h \) is normally time-independent in the physical limit, and each \( M^0 \) can then be evaluated directly. For example, when \( h(r) = 0 \),

\[
M^0_1 \left( r_i t_i \right) = \langle t_a(r, t) \rangle = 0,
\]

\[
M^0_2 \left( r_i t_i t_j \right) = \langle (t_a(r, t_i) t_a(r, t_j) t_a(r, t_k)) \rangle - \langle t_a(r, t_i) \rangle \langle t_a(r, t_j) \rangle \langle t_a(r, t_k) \rangle
\]

\[
= \frac{\delta(x_1 x_2)}{3} \left( 1 + \frac{1}{s} \right),
\]

0, unless \((x_1 x_2 x_3)\) are some permutation of \((xyz)\),

\[
M^0_3 \left( r_i t_i t_j t_k \right) = \begin{cases} 
\frac{(+i)}{6s} \left( 1 + \frac{1}{s} \right), \text{ for time orderings giving } (xyz) \\
\frac{(-i)}{6s} \left( 1 + \frac{1}{s} \right), \text{ for time orderings giving } (yzy) \\
\text{cyclic permutations.}
\end{cases}
\]

When \( h = 0 \), \( M^0 \) is constant for any given time ordering and the evaluation reduces to finding traces of spin-operator products. The presence of a time-independent non-zero field makes things only marginally more complicated. Relevant traces have been evaluated to high order by Dalton and Rimmer (1968).

It is sometimes convenient to have equations of motion for the \( M^0 \)s. When \( v = 0 \),

\[
i \frac{\partial}{\partial t} t_a = [t_a, H] = (-i) \sum_{\beta} e^{\gamma} H_{\beta} t_{\gamma},
\]

where \( e^{\gamma} \) is the completely antisymmetric matrix,

\[
e^{\gamma} = \begin{cases} 
1, \text{ when } x\beta \gamma \text{ is a cyclic permutation of } xyz \\
-1, \text{ when } x\beta \gamma \text{ is a cyclic permutation of } yzx \\
0, \text{ otherwise.}
\end{cases}
\]

Thus, for example,

\[
\sum_{\gamma}(G_0^{-1}(t_i))^{\gamma} M^0_2 \left( r_i t_i t_j \right) = -\frac{\delta(t_i t_j)}{s} \sum_{\gamma} e^{\gamma} M^0_1 \left( r_i t_i \right)
\]

where

\[
(G_0^{-1}(t))^{\gamma} \equiv \delta^{\gamma} i \frac{\partial}{\partial t} + i \sum_{\beta} e^{\beta} H_{\beta} t_{\gamma}.
\]

The general form is, schematically,

\[
G_0^{-1} M^0_n = \frac{1}{s} \sum_{n-1} M^0_n \delta,
\]

which can help to evaluate those parts of the semi-invariants that are not time-independent. In the classical limit \( s \to \infty \), the semi-invariants become entirely time-independent and go over into their classical forms (149), (150).

Unrenormalised perturbation theory for the Heisenberg model has been developed by Stinchcombe et al. (1963) and by Vaks et al. (1968a, b). To develop \( W \) in powers of \( v \), there are as usual two routes. Either we directly expand the time-ordered exponential \( U \) (Englert, 1963) (cf. Section II.C) or we use (163) to generate the coefficients in the Taylor expansion (cf. (11) and (12)). It is clear from either point of view that each potential line \( v \) carries a factor \( i \) and requires a time integral over the interval \([0, -i\beta]\). Otherwise, the topology of the development parallels exactly Sections II.B, II.C, and III.C.

The result is

\[
W = \sum_{\text{all topologically distinct unrooted}} \begin{cases} 
\text{connected graphs according to Rule 18.} \\
\end{cases}
\]

**Rule 18: Heisenberg Model Free Energy W, Unrenormalised Form**

(a) Assign to each vertex a dummy spatial label \( \bar{r} \). Assign to each edge a Cartesian index \( \gamma \) and a time variable \( t \).

(b) For each edge labeled \( \gamma, t \) and joining vertices \( \bar{r}_1 \) and \( \bar{r}_2 \), write a factor \( iv^\gamma (\bar{r}_1, \bar{r}_2) \).

(c) For each \( \gamma \)-valent vertex \( r \) with incident edges \( \gamma_1 t_1, \ldots, \gamma_n t_n \), write a factor

\[
M^0_\gamma \left( \bar{r}, \gamma_1 t_1, \ldots, \gamma_n t_n \right).
\]

(d) Sum each internal vertex label freely over the entire lattice. Integrate each time variable \( \int_0^{i\beta} dt \). Sum each Cartesian index \( \gamma = x, y, z \).

(e) Divide by the symmetry factor of the unrooted graph.

The first few contributing graphs are given by (20). Note that in the classical limit each time integral provides a factor \((-i\beta)\) which combines with \((iv)\) to form \( \beta v \) which was called \( v \) in III.C. It is also possible (and convenient when \( v \) is isotropic) to use a spherical representation, \( t_i, t_-, t_+ \).
The correlation functions (161) are derived by differentiation. For example,

\[ M_{\alpha\beta}(12) - \delta(r_1, r_2)M_2(r_1, r_2, R) = \sum \text{ (sum of all topologically distinct) 2-rooted connected graphs} \text{ according to Rule 19).} \]  

(171)

**Rule 19: Heisenberg Model Pair Correlations, Unrenormalised Form**

(a) Assign to each internal vertex a dummy spatial label \( \bar{r} \). Assign to each edge a Cartesian index \( \gamma \) and a time variable \( t \). Assign to the external vertices 1 and 2 the labels \( r_1, t_1 \) and \( r_2, t_2 \).

(b) For each edge labeled \( \gamma, t \) and joining vertices \( \bar{r}_1 \) and \( \bar{r}_2 \), write a factor \( iv^\gamma(r_1, r_2) \).

(c) For each \( l \)-valent internal vertex \( \bar{r} \) with incident edges \( \gamma_1, t_1, \ldots, \gamma_l, t_l \), write a factor

\[ M_1^l(\bar{r}, \gamma_1, t_1, \ldots, \gamma_l, t_l). \]

For each \( l \)-valent external vertex \( i = 1, 2 \), write a factor

\[ M_{i+1}^0(r_i, \gamma_i, t_i). \]

where \( \gamma = \alpha(\beta) \) if \( i = 1(2) \).

(d) Sum each internal vertex label freely over the entire lattice. Integrate each internal time \( [0, -i\beta] \). Sum the Cartesian index of each edge \( \gamma = x, y, z \).

(e) Divide by the symmetry factor of the 2-rooted graph.

Graphs are given by (30). For example,

\[ \frac{1}{2} \beta \cdot \bar{r} \left( \sqrt{2} \sum_{\gamma_1, \gamma_2} \int_0^{-i\beta} d\gamma_1 d\gamma_2 \nabla_{r_1}^\gamma(r_1) \nabla_{r_2}^\gamma(r_2, t_2) M_2(\bar{r}, \gamma_1, \gamma_2, t_1, t_2) \right) \]

\[ \times M_2(\bar{r}, \gamma_1, \gamma_2, t_1, t_2) M_2(\bar{r}, \gamma_1, \gamma_2, t_1, t_2). \]  

(172)

The first few terms of the Heisenberg model correlations have been evaluated by another method by Tahir-Kheli and McFadden (1969) and McFadden and Tahir-Kheli (1970a, b).

Renormalisation is straightforward. In calculating insertions such as the self-field \( G \) the external vertex takes a factor 1 and the \( \gamma, t \) labels of all edges incident at it remain unsummed. Renormalisation proceeds as previously (cf. (42), (154)),

\[ M_n(r_1, \ldots, t_n) = \exp \sum_{i=1}^n (-i)^i \int_0^{-i\beta} d\gamma_1 \ldots d\gamma_i \sum_{\gamma_1, \ldots, \gamma_i} G_i(r_1, \gamma_1, \ldots, \gamma_i, t_1, \ldots, t_i) \]

\[ \times \frac{\delta}{\delta h_0^\gamma(r_1, \gamma_1) \ldots \delta h_0^\gamma(r_i, \gamma_i)} M_n(\bar{r}, \gamma_1, \ldots, \gamma_i). \]  

(173)

The analog of the many-particle Dyson equation is made most evident by applying \( \mathcal{G}^{-1}_0 \) to (173). The result in rather schematic form is (cf. (169)),

\[ \mathcal{G}^{-1}_0 M_n = \frac{1}{s} \sum_{n-1} M_{n-1} + \frac{1}{s} \sum_{n+1} G_i M_{n+1}. \]  

(174)

Renormalisation has not been carried out systematically in the literature beyond the molecular field approximation, \( \Phi = \frac{1}{2} \int \phi^2 \). Better approximations based on (174) seem to give high-temperature results similar to Résibois and De Leeer (1966, 1969) and De Leeer and Résibois (1966, 1969).

**E. Fermion variables**

The only complications produced by the introduction of fermion variables are sign factors. In the fourth of his papers on what is now known as the Hubbard model, Hubbard (1965) has developed the unrenormalised perturbation theory for the fermion Hamiltonian,

\[ \mathcal{H} = \sum_{r_1, r_2} t(r_1, r_2) a_{\sigma}^+ (r_1) a_{\sigma}(r_2) + I \sum_{r_1} n_{\sigma}(r_1) n_{\sigma}(r_1), \]  

(175)

\( (n_{\sigma} = a_{\sigma}^+ a_{\sigma}) \) where \( I \) represents an intratomic coulomb repulsion and \( t(r_1, r_2) \) is an interatomic hopping integral. To use the methods we have developed, one regards the second term in (175) as the (spatially local) non-interacting Hamiltonian and expands in powers of the kinetic energy. In order to have the freedom of functional methods it is necessary to introduce anticommuting fields (Schwinger, 1951) which couple directly to the fermion creation and destruction operators,

\[ \mathcal{H}'(t) = \sum_{r, \sigma} \xi_{\sigma}(r, t) a_{\sigma}(r, t) + \eta_{\sigma}(r) a_{\sigma}^+ (r, t). \]  

(176)

The reader is referred to Hubbard’s work for further details. Renormalisation has not yet been used.
Appendix: The Relation of the Free Multiplicities to the Weak Lattice Constants

Part (d) of all linked-cluster-expansion rules requires for a given graph the summation of a number of terms, each one associated with a specific realisation of that graph on the underlying lattice, i.e. with a specific assignment of each graphical vertex to a given lattice site. When interactions are uniform, isotropic in the lattice, and restricted to nearest neighbors (e.g. (21), (23)), all terms in such a summation are identical. In such a situation the total contribution of the graph is the value of any one term times the number of terms. The number of terms is called the free multiplicity.

We confine our main discussion to unrooted graphs for the sake of simplicity. For specificity we shall always take the underlying lattice to be large and toroidally connected. An embedding of a graph \( G \) in a lattice is an assignment of the graph vertices to the sites of the lattice in such a way that all graph edges lie along nearest-neighbour bonds of the lattice. Free embedding allows several distinct graph vertices to be assigned to the same lattice site. Weak embedding allows no more than one vertex to be assigned to each site. The free multiplicity \( m(G) \) of an unrooted graph \( G \) on a given lattice is the number of distinct free embeddings of the labelled graph \( G \) (i.e. the vertices are regarded as distinguishable) in the lattice per site of the lattice. The weak lattice constant \( p(G) \) of the unrooted graph \( G \) in the lattice is the number of distinct weak embeddings of the unlabelled graph \( G \) in the lattice per site of the lattice. We show below that \( m(G) \) and \( p(G) \) are closely related.

We assert that for a given lattice:

(i) For a properly chosen set of graphs \( G \in S \), \( m(G) \) is related to \( p(G) \) by a conversion matrix \( A \) (Sykes et al., 1966),

\[
m(G) = \sum_{G' \in S} A(G(G')) p(G'), \quad A(G(G')) \geq 0.
\]

(ii) \( A \) is a non-singular matrix and can therefore be inverted, giving the weak lattice constants \( p \) in terms of the \( m \)'s.

Note first of all that any graph with multiple edges has the same embeddings as the corresponding reduced graph in which all multiple edges have been replaced by single edges. We therefore restrict attention to graphs having only single edges.

Define a collapse of a graph \( G \) as a graph formed from \( G \) by (a) identifying (figuratively, “gluing together”) previously distinct vertices of \( G \); and (b) reducing all multiple edges thus formed. The graph \( G \) and all its collapses form the collapse chain of \( G \). The members of the collapse chain of \( G \) can be ordered (in general, in a variety of ways), \( G = G_1, G_2, \ldots, G_n, \) so that no graph \( G_i \) collapses into any graph to its left \( (i < n) \). Such an ordering is a standard ordering. The collapse chain of the graph \( G \) is shown in Fig. 16. The collapse matrix \( C(G(G')) \geq 0 \) is the number of distinct ways in which the labelled graph \( G \) collapses into the unlabelled graph \( G' \).

![Fig. 16. A collapse chain arranged in standard order.](image)

In the process of counting the free multiplicity of \( G \), all collapses \( G' \) are included. Each collapse \( G' \) has \( g(G') p(G') \) labelled weak embeddings per site of the lattice. Thus,

\[
m(G) = \sum_{G'} C(G(G')) g(G') p(G'),
\]

where the sum is over the graphs in the collapse chain of \( G \). This proves (i). The matrices \( C \) and \( A \) for the collapse chain shown in Fig. 16 are given below.

\[
A = \begin{bmatrix}
1 & 1 & 2 & 2 & 3 & 3 & 4 & 1 \\
1 & 0 & 0 & 0 & 2 & 2 & 1 \\
1 & 0 & 2 & 0 & 0 & 0 \\
1 & 1 & 0 & 2 & 1 & 1 \\
1 & 0 & 0 & 0 & 0 & 0 \\
1 & 3 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1
\end{bmatrix}
\]

\[
C = \begin{bmatrix}
2 & 8 & 4 & 4 & 18 & 6 & 8 & 2 \\
8 & 0 & 0 & 0 & 4 & 2 \\
2 & 0 & 1 & 2 & 0 & 0 & 0 \\
2 & 6 & 0 & 4 & 2 \\
6 & 0 & 0 & 0 & 0 \\
6 & 4 & 2 \\
2 & 2 \\
2 & 2
\end{bmatrix}
\]  \hspace{1cm} (A.2)

To prove part (ii) of the original assertion note that, when the collapse chain of \( G \) is arranged in standard order, both \( C \) and \( A \) are triangular. All diagonal elements are positive, so \( \det A \neq 0 \) and \( A^{-1} \) exists.

There is no difficulty in extending the above to sets of graphs formed by taking the union of two or more collapse chains.

The free multiplicity of an \( n \)-rooted graph \( G \) on a given lattice is the number of free embeddings of the labelled graph \( G \) in the lattice subject to the condition that the external vertices are fixed on the lattice sites \( r_1, \ldots, r_n \).

† The weak lattice constants are closely related to the strong lattice constants and derivable from them, as shown by Sykes et al. (1966). See Domb this volume, Chapter I, Section IV.

‡ No “loops” (i.e. edges with both ends at the same vertex) may be formed in this process.
The simplifying feature of the free multiplicities (relative, for example, to the weak or strong lattice constants) is that different parts of the graph do not interfere with one another, since they can interpenetrate on the lattice. Thus, the free multiplicities are larger than the weak or strong lattice constants but often far easier to evaluate. For example, the free multiplicity of the unrooted chain of $n$ links is just $q^n$ ($q = $ coordination number). Similarly the free multiplicity of a 1-rooted graph whose external vertex is an articulation point is just the product of the free multiplicities of the associated 1-insertions. These and other related observations are discussed by Jansow (1969). They are incorporated in a natural way into the renormalisations we have performed in the text.

References


4. Asymptotic Analysis of Coefficients

D. S. Gaunt and A. J. Guttmann†

Wheatstone Physics Laboratory, King’s College, University of London, England

I. Introduction ........................................ 181
A. General problem .................................. 181
B. Basic properties of power series .............. 184
C. Comment on content ............................. 186

II. Ratio Method ........................................ 187
A. Preliminary estimates ......................... 187
B. Neville tables ..................................... 191
C. Refined estimates ............................... 192
D. Loose-packed lattices ......................... 195
E. Extrapolation formulae ....................... 199

III. Padé Approximants .............................. 202
A. Background ....................................... 202
B. Theory ........................................... 203
C. Padé method ..................................... 206
D. Applications ..................................... 210

IV. Method of N Point Fits .......................... 219
V. Transformations of Expansion Variables .... 224
VI. Applications of Darboux’s Theorems .......... 232
A. Introduction ..................................... 232
B. Close-packed lattices ......................... 232
C. Loose-packed lattices ......................... 234
D. Contour map method ......................... 238

Acknowledgments .................................. 241
References .......................................... 241

I. Introduction

A. General problem

It can been seen in other chapters of this volume how power series expansions may be developed for various lattice models in any dimension. The expansions are exact as far as they go, and clearly represent a good deal of

† Present address: Department of Mathematics, University of Newcastle, New South Wales, Australia 2308.