charged Co^{57} is present as Fe^{++} only. This is to be contrasted with NaCl where both Fe^{+} and Fe^{+++} are observed.[29]

(c) There is a noticeable degree of covalency in the binding of Fe^{++} in AgCl.

(d) The effect of the variation in fluctuation time of an EFG have been observed for the first time in the Mössbauer effect.

(e) The silver-ion-vacancy jump times are much faster than those of alkali-ion vacancies in the alkali halides (about 10^5 faster at room temperature). These jump times are apparently largely independent of the identity of impurity.

[29] J. G. Mullen, Phys. Rev. **131**, 1415 (1963).

ACKNOWLEDGMENTS

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Ising-Model Reformulation. III. Quadruplet Spin Averages

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A previously developed method for diagrammatic expansion of the Ising-model partition function and pair distribution function is applied to calculation of the field-free quadruplet spin averages $\langle\mu_1\mu_2\mu_3\mu_4\rangle$. The central four-vertex function Q generated by these averages is topologically analyzed in standard fashion in terms of an irreducible four-vertex quantity e. Several rigorously necessary conditions that must be satisfied by Q are listed. It is furthermore pointed out that the existence of a logarithmic specific-heat anomaly puts an additional constraint on quadruplet averages (which is verified in an Appendix by direct calculation on the Ising-Onsager two-dimensional square lattice). Upon making a simplifying functional assumption for Q, this latter quantity may be entirely determined above T_c by one of the necessary conditions. This leads at T_c to a $k^{d/2}$ spectrum (d=dimensionality) and above T_c to a logarithmic specific heat, both of which were adduced by Abe's Ising-model version of the He^4 speculative analysis due to Patashinskii and Pokrovskii (but for different reasons from those in the present analysis). Sinec the Abe-Patashinskii-Pokrovskii spectrum almost certainly exhibits an incorrect exponent, an alternative and more powerful functional assumption for Q is suggested which still yields a soluble theory in principle, but construction of the solution is not attempted here.

I. INTRODUCTION

In a previous article,[1] some of the techniques of quantum field theory were employed to generate a diagram expansion for the general Ising-model partition function $Z(\beta)$ and low-order spin averages. The partition function was expressed as a vacuum-state expectation value of the product of two operators:

$$Z(\beta)=\langle 0|\exp(-\beta\mathbf{M})\exp(\mathbf{D}^\dagger)|0\rangle, \quad \beta=(k_BT)^{-1}, \quad (1)$$

and the "vacuum" may be regarded as a set of unexcited one-dimensional harmonic oscillators, one at each lattice site. Operators $\mathbf{M}$ and $\mathbf{D}^\dagger$ can be expressed in terms of the canonical boson field operators $\mathbf{b}(\mathbf{k})$ and $\mathbf{b}^\dagger(\mathbf{k})$:

$$M=\sum_{\mathbf{k}}^{(\tau)}\{H(-\mathbf{k})\mathbf{b}^\dagger(\mathbf{k})+H(\mathbf{k})\mathbf{b}(\mathbf{k}) +V(\mathbf{k})[\tfrac{1}{2}\mathbf{b}^\dagger(\mathbf{k})\mathbf{b}^\dagger(-\mathbf{k})+\mathbf{b}^\dagger(\mathbf{k})\mathbf{b}(\mathbf{k}) +\tfrac{1}{2}\mathbf{b}(\mathbf{k})\mathbf{b}(-\mathbf{k})]\}; \quad (2)$$

[1] F. H. Stillinger, Jr., Phys. Rev. **135**, A1646 (1964).

$$\mathbf{D}^\dagger=\sum_{n=2}^{\infty}N^{1-n}D_n\sum_{\mathbf{k}_1\cdots\mathbf{k}_{2n-1}}^{(\tau)}\mathbf{b}^\dagger(\mathbf{k}_1)\cdots\mathbf{b}^\dagger(\mathbf{k}_{2n-1}) \times\mathbf{b}^\dagger(-\mathbf{k}_1-\cdots-\mathbf{k}_{2n-1}). \quad (3)$$

Here, $H(\mathbf{k})$ and $V(\mathbf{k})$ are the discrete-lattice Fourier transforms of the external field $h(\mathbf{r})$ and the pair potential $v(\mathbf{r})$, and the $\mathbf{k}$'s are the reciprocal lattice vectors, confined to the first Brillouin zone τ. The numerical coefficients D_n may be expressed as the following integrals:

$$D_n=\frac{(-1)^{n-1}2^{2n}}{\pi^{2n}(2n)!}\int_0^\infty\frac{y^{2n-1}dy}{\sinh y}, \quad (4)$$

or alternatively written in terms of Bernoulli numbers.

In Ref. 1 it was convenient to consider the operators $\exp(\mathbf{D}^\dagger)$ and $\exp(-\beta\mathbf{M})$ in Eq. (1) to act, respectively, during "time" intervals of unit length and length β. Time ordering of operators, followed by operator contractions in accord with Wick's theorem then generated the requisite diagrams.

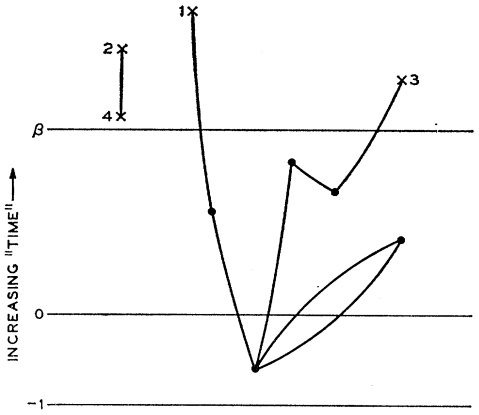

FIG. 1. Diagram of a process contributing to the spin-quadruplet average, Eq. (6). Bursts of an even number of excitations (≥ 4) due to $\mathbf{D}\dagger$ occur in the lower strip, and for vanishing external field only pair vertices from $\mathbf{M}$ appear in the upper strip.

Spin averages may be obtained from $\ln Z(\beta)$ by differentiation with respect to external field intensity at the sites involved. Diagrammatically, each such differentiation provides a root point for the spin-average diagrams. It was previously found that the set of doubly rooted graphs contributing to the pair correlation function in the absence of external fields could formally be summed to yield[2,3]

$$\langle \mu_1 \mu_2 \rangle \equiv \psi(\mathbf{r}_{12},\beta) = -\frac{1}{\tau}\int_\tau d\mathbf{k}\, \Psi(\mathbf{k},\beta) \exp(-i\mathbf{k}\cdot\mathbf{r}_{12}),$$
$$\Psi(\mathbf{k},\beta) = \frac{[1+W(\mathbf{k},\beta)]}{1+[1+W(\mathbf{k},\beta)]\beta V(\mathbf{k})}. \tag{5}$$

The function $W(\mathbf{k},\beta)$ is analogous to a proper self-energy, in that its diagrammatic basis involves divergence into several parallel routes from the original path connecting the roots of the ψ diagram, then convergence to a single path again.

Calculation of $W(\mathbf{k},\beta)$ then forms the central problem in the present reformulation. In particular the singular nature of this function at the critical point $\beta=\beta_c$ holds they key to understanding critical phenomena. It is one of the central aims in this paper to study W through the β differential equation for ψ. Since this latter equation involves quadruplet spin averages, we are motivated to study in detail the set of quadruply rooted diagrams which will quantitatively be specified in the following Sec. II, and then subjected to standard topological reductions in Sec. III.

The difficulty of evaluating any but the simplest class of diagrams in a many-body theory is of course well known. With a view to eliminating to some extent these difficult evaluations, we display a set of necessary conditions (Sec. V) on the primary four-vertex diagram sum, denoted below by Q. To illustrate the utility of these restrictions, it is shown in Sec. VI that for $\beta \leq \beta_c$ a simple functional assumption on Q leads to an implicitly soluble "model," exhibiting similar behavior in the critical region to that obtained by Abe,[4] with complete elimination of the need to evaluate any diagrams whatever. To the extent that W is the two-vertex analog of Q, and that a similar functional assumption on W which suppresses $\mathbf{k}$ dependence across τ leads to the spherical model[5,6] as shown in Ref. 1, we obtain here a result representing in some ways a natural step beyond the spherical model.

The quadruplet averages naturally also appear in the rigorous specific-heat expression, since this thermodynamic quantity is related to fluctuations of the interaction energy. Section IV points out the implications for W and Q for logarithmic specific heat anomalies known for two-dimensional models,[7] and often suspected in three dimensions.[8]

II. SPIN QUADRUPLET DIAGRAMS

We briefly sketch the adaptation to quadruplet spin averages of the argument given in Ref. 1 leading to diagram expansion. The starting point is a vacuum-state matrix-element expression corresponding to Eq. (1)[9]:

$$\langle \mu_1\mu_2\mu_3\mu_4 \rangle = N^{-2}Z^{-1}(\beta) \sum_{\mathbf{k}_1\cdots\mathbf{k}_4}^{(\tau)} \langle 0 | \prod_{j=1}^{4} [\exp(-i\mathbf{k}_j\cdot\mathbf{r}_j)\mathbf{b}^\dagger(\mathbf{k}_j) + \exp(i\mathbf{k}_j\cdot\mathbf{r}_j)\mathbf{b}(\mathbf{k}_j)] \times \exp(-\beta\mathbf{M}) \exp(\mathbf{D}^\dagger) | 0 \rangle. \tag{6}$$

The set of contributions to (6) may be graphed as before on a pair of parallel strips, width β and 1 for "time"-ordered operation of $\mathbf{M}$ and $\mathbf{D}^\dagger$, respectively, as shown in Fig. 1. Vertical direction in the Figure corresponds to reading right-to-left in the operator product in Eq. (6); consequently the four root points corresponding to the four spins appear at the top.

The contributions to (6) are of various types according to how (or indeed whether) they connect the four root points. Those unconnected to the roots are cancelled by the $Z(\beta)$ division. Contributions whose diagrams connect the roots in pairs yield the following sum of products of pair correlation functions:

$$\psi(\mathbf{r}_{12})\psi(\mathbf{r}_{34}) + \psi(\mathbf{r}_{13})\psi(\mathbf{r}_{24}) + \psi(\mathbf{r}_{14})\psi(\mathbf{r}_{23}). \tag{7}$$

[2] $\mathbf{k}$-space sums in the infinite system limit pass to integrals in the manner:

$$N^{-1}\sum_{\mathbf{k}}^{(\tau)} \to \frac{1}{\tau}\int_\tau d\mathbf{k}.$$

[3] An alternative means of obtaining this result may be found in J. L. Lebowitz, G. Stell, and S. Baer, J. Math. Phys. 6, 1282 (1965) [see Eq. (5.25)].

[4] R. Abe, Progr. Theoret. Phys. (Kyoto) 33, 600 (1965).
[5] T. H. Berlin and M. Kac, Phys. Rev. 86, 821 (1952).
[6] H. W. Lewis and G. H. Wannier, Phys. Rev. 88, 682 (1952).
[7] L. Onsager, Phys. Rev. 65, 117 (1944).
[8] M. E. Fisher, J. Math. Phys. 4, 278 (1963).
[9] Some transformations of such matrix elements are given in F. H. Stillinger, Jr., Phys. Rev. 138, A1174 (1965).

Diagrams for remaining terms have all four roots mutually connected through vertices within the strips, which are also connected among themselves; an example is shown in Fig. 2.

At this stage it is convenient to carry out certain partial diagram summations. It may first be noted from Figs. 1 and 2 that vertices in the bottom strip, arising from $\mathbf{D}^\dagger$, may have loops attached to them which have no other points of attachment to the diagram. A formal summation over all such loops at a given lower-strip vertex has the effect of "renormalizing" each constant D_n in Eq. (4) to a temperature-dependent value $\bar{D}_n(\beta)$.[10] Secondly, each diagram of the connected variety illustrated in Fig. 2 consists of "arms" from each of the roots entering a four-terminal complex (merely a point in Fig. 2). Figure 3 indicates in abbreviated form the diagram in Fig. 2, with only the distinguished four-terminal vertex and the roots shown for convenience.

Indeed, we shall regard Fig. 3 as standing for the sum of the entire set of graphs of the type shown in Fig. 2, including renormalization of the central vertex. In obtaining an explicit representation of the sum for Fig. 3, we recognize that each arm might directly have entered the distinguished vertex, or have done so after passing through any number of V and W processes *provided* that the last process before entering the distinguished vertex was a V, not a W. Hence each arm summation generates a "bond" or "propagator,"[11]

$$T(\mathbf{k},\beta)=1/\{1+[1+W(\mathbf{k},\beta)]\beta V(\mathbf{k})]\}, \quad (8)$$

similar to the pair correlation transform $\Psi(\mathbf{k},\beta)$. As a result, the $\mathbf{k}$-space form of the contribution of Fig. 3 is

$$4!T(\mathbf{k}_1,\beta)T(\mathbf{k}_2,\beta)T(\mathbf{k}_3,\beta)T(-\mathbf{k}_1-\mathbf{k}_2-\mathbf{k}_3,\beta)\bar{D}_2(\beta), \quad (9)$$

where the 4! arises from all possible assignments of $\mathbf{D}^\dagger$ operators to the four distinguishable arms, under operator contractions (which require momentum conservation) during the original diagram generation.

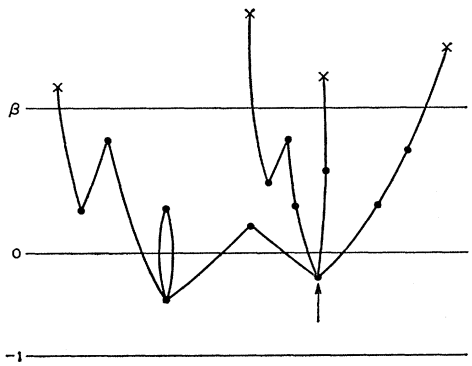

FIG. 2. Spin-quadruplet diagram in which the four root points are mutually connected through strip vertices. The arrow indicates the distinguished point receiving the four arms.

[10] Details are given in Ref. 1. The precise values of the renormalized constants are irrelevant in the remainder of this paper.

[11] Expansion of Eq. (8) reproduces the sequence of W's and V's that are allowed along an "arm."

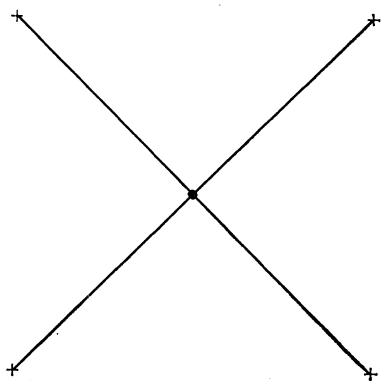

FIG. 3. Abbreviated diagram for the sum of terms of the type shown in Fig. 2. Summation has been carried out over all possible "arms," and over loops attached to the distinguished vertex, which therefore has attached to it the renormalized value $\bar{D}_2(\beta)$.

The single remaining vertex after diagram abbreviation is but the simplest case of an infinite variety of four-terminal complexes receiving the root arms. Figure 4 displays a few of the possibilities. These complexes all possess renormalized vertices of even order connected by internal bonds, along which partial summations will be presumed already performed. Since in this case a V necessarily lies next to each explicitly indicated vertex, the appropriate internal bond stands for the propagator:

$$L(\mathbf{k},\beta)=-\beta V(\mathbf{k})/\{1+[1+W(\mathbf{k},\beta)]\beta V(\mathbf{k})\}. \quad (10)$$

Of course momentum conservation still applies at each renormalized vertex.

The totality of four-terminal complexes defines the four-terminal function Q, as shown symbolically in Fig. 4. Therefore, setting

$$\langle\mu_1\mu_2\mu_3\mu_4\rangle-\psi(\mathbf{r}_{12})\psi(\mathbf{r}_{34})-\psi(\mathbf{r}_{13})\psi(\mathbf{r}_{24})-\psi(\mathbf{r}_{14})\psi(\mathbf{r}_{23}) \equiv\psi^{(4)}(\mathbf{r}_{12},\mathbf{r}_{13},\mathbf{r}_{14}), \quad (11)$$

the Fourier transform of $\psi^{(4)}$ is

$$\Psi^{(4)}(\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4)=T(-\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}_4) \times T(\mathbf{k}_2)T(\mathbf{k}_3)T(\mathbf{k}_4)Q(\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4). \quad (12)$$

The conservation of momentum for the propagators entering the four terminals of Q reinforces the temptation to regard this function as a scattering amplitude for boson spin excitations. The major object in the present development then becomes determination of this scattering amplitude, and understanding of its role in the domain of critical phenomena.

III. TOPOLOGICAL REDUCTIONS

After careful attention has been directed to the combinatorial factors inherent in operator contractions in Eq. (6), the amplitude Q may explicitly be written

out as a sum over permissible four-terminal diagrams $\mathbf{R}$:

$$Q(\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4,\beta)=\sum_{\{R\}}[\sigma(\mathbf{R})]^{-1}[4!N^{-1}\tilde{D}_2(\beta)]^{n_2(\mathbf{R})}\cdots \times[(2l)!N^{1-l}\tilde{D}_l(\beta)]^{n_l(\mathbf{R})}\cdots \times\sum_{\mathbf{k}_1'\cdots\mathbf{k}_{\mu(R)}'}{}^{(\tau)\prime}\sum_{\alpha=1}^{\mu(\mathbf{R})}L(\mathbf{k}_\alpha',\beta). \quad (13)$$

In this expression, the momenta along the $\mu(\mathbf{R})$ internal diagram bonds L are $\mathbf{k}_\alpha'$, and the $n_l(\mathbf{R})$ are the numbers of renormalized vertices at which $2l$ bonds (internal or external) converge. The diagram symmetry number is $\sigma(\mathbf{R})$. The primed momentum summation enforces momentum conservation at each vertex, including the four terminals with their external T-bond momenta.

The structure of the infinite diagram set $\{\mathbf{R}\}$ may at least be partially revealed by a topological reduction to an irreducible four-terminal function, in exactly the same manner as has been done in the regime of the quantum-mechanical many-body problem[12]; we repeat the argument here for completeness. It is perhaps easiest to visualize the subsequent relations in their direct space representation, so let $q(\mathbf{r}_{12},\mathbf{r}_{13},\mathbf{r}_{14})$ be the $\mathbf{r}$-space four-terminal function whose transform with respect to the three relative position variables is $Q(\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4)$

$$Q(\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4)=\sum_{\mathbf{r}_{12},\mathbf{r}_{13},\mathbf{r}_{14}}\exp[i(\mathbf{k}_2\cdot\mathbf{r}_{12}+\mathbf{k}_3\cdot\mathbf{r}_{13}+\mathbf{k}_4\cdot\mathbf{r}_{14})]\times q(\mathbf{r}_{12},\mathbf{r}_{13},\mathbf{r}_{14}). \quad (14)$$

It is convenient to introduce an auxilliary four-terminal function $c(\mathbf{r}_{12},\mathbf{r}_{13},\mathbf{r}_{14})$, which stands for a subset of the entire diagram set $\{\mathbf{R}\}$. The diagrams of the c set are those which cannot be separated, by cutting precisely two internal bonds, into two portions, one of which contains terminals 1 and 2, the other containing 3 and 4. The simplest members of the c set are shown in Fig. 5. Note from the figure that *some* of the diagrams in the subset *could* nevertheless be so bisected into parts

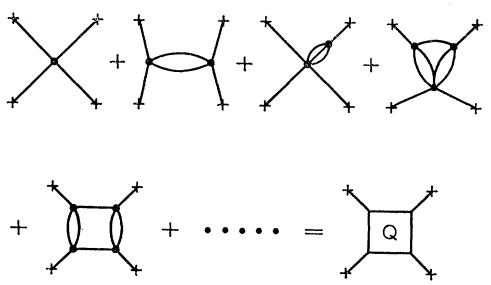

FIG. 4. Definition of Q as the sum of all four-terminal complexes. The incoming bonds from the roots to the four terminals have been included for completeness.

[12] A. Z. Patashinskii and V. L. Pokrovskii, Zh. Eksperim. i Teor. Fiz. **46**, 994 (1964) [English transl.: Soviet Phys.—JETP **19**, 677 (1964)].

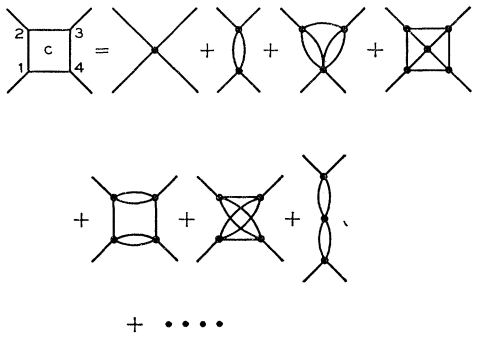

FIG. 5. Some simple diagrams contributing to the auxilliary four-terminal function c.

containing, respectively, terminal pairs (13) and (24), or (14) and (23).

The original function q may easily be reconstructed from c as shown in Fig. 6. The point is that those diagrams in $\{\mathbf{R}\}$ which permit two-bond cuts leading to (12), (34) separation, consist of a string of c-type contributions connected by parallel pairs of bonds. The infinite series of such strings of arbitrary numbers of c nodes obviously may be summed by the integral equation

$$q(\mathbf{r}_{12},\mathbf{r}_{13},\mathbf{r}_{14})=c(\mathbf{r}_{12},\mathbf{r}_{13},\mathbf{r}_{14})+\sum_{\mathbf{r}_5\ldots\mathbf{r}_8}c(\mathbf{r}_{12},\mathbf{r}_{15},\mathbf{r}_{16})l(\mathbf{r}_{58})l(\mathbf{r}_{67})\times q(\mathbf{r}_{78},\mathbf{r}_{73},\mathbf{r}_{74}), \quad (15)$$

$$L(\mathbf{k},\beta)=\sum_{\mathbf{r}}\exp(i\mathbf{k}\cdot\mathbf{r})l(\mathbf{r},\beta),$$

which is also exhibited in Fig. 6. Relation (15) constitutes a four-terminal version of the Ornstein-Zernike integral equation connecting fluid pair and direct correlation functions.[13]

The quantity $c(\mathbf{r}_{12},\mathbf{r}_{13},\mathbf{r}_{14})$ is not a completely symmetric function of its argument vectors as is $q(\mathbf{r}_{12},\mathbf{r}_{13},\mathbf{r}_{14})$, on account of the unsymmetrical manner of treating the four terminals in its definition. However, c is symmetric with respect to interchange of its last two arguments. Consider the symmetric sum

$$s(\mathbf{r}_{12},\mathbf{r}_{13},\mathbf{r}_{14})=c(\mathbf{r}_{12},\mathbf{r}_{13},\mathbf{r}_{14})+c(\mathbf{r}_{13},\mathbf{r}_{12},\mathbf{r}_{13})+c(\mathbf{r}_{14},\mathbf{r}_{12},\mathbf{r}_{13}). \quad (16)$$

Those diagrams in $\{\mathbf{R}\}$ which allow separation by scission of two bonds will appear twice, those which do not will appear three times. The diagram subset for the latter may be termed "irreducible," and the corresponding four-terminal function denoted by e. Then subtracting e from s produces each member of $\{\mathbf{R}\}$ twice, i.e.,[14]

$$q(\mathbf{r}_{12},\mathbf{r}_{13},\mathbf{r}_{14})=\tfrac{1}{2}[c(\mathbf{r}_{12},\mathbf{r}_{13},\mathbf{r}_{14})+c(\mathbf{r}_{13},\mathbf{r}_{12},\mathbf{r}_{14})+c(\mathbf{r}_{14},\mathbf{r}_{12},\mathbf{r}_{13})-e(\mathbf{r}_{12},\mathbf{r}_{13},\mathbf{r}_{14})]. \quad (17)$$

[13] L. S. Ornstein and F. Zernike, Koninkl. Ned. Akad. Wetenschap. Proc. **17**, 793 (1914).

[14] Substantially the same relation appears in both Ref. 4 and Ref. 12.

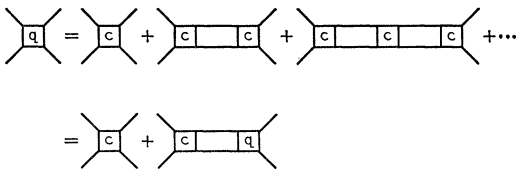

FIG. 6. Generation of the set {R} of diagrams for q out of the c set.

Some of the leading contributions to the symmetric function e are graphed in Fig. 7. The inherent difficulty in the general Ising problem thus has been transferred to determination of e, for once this function is given, Eqs. (15) and (17) together would self-consistently determine c and q, and from the latter the pair correlation function and thermodynamic properties of the model could subsequently be deduced.

IV. SPECIFIC HEATS

It is now appropriate to record a few heuristic observations about the temperature dependence of $W(\mathbf{k},\beta)$ and $Q(\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4,\beta)$ with particular emphasis on infinite specific heat anomalies at the critical point ($\beta=\beta_c$).

The phase transition at β_c is heralded by the occurrence of an infinity somewhere in τ of the $\mathbf{k}$-dependent susceptibility $\Psi(\mathbf{k},\beta)$, Eq. (5). In the case of ferromagnetic interactions[15] for which $V(\mathbf{k})$ possesses an absolute minimum at $\mathbf{k}=0$, this singularity will result from first occurrence of a zero (at $\mathbf{k}=0$) of Ψ's denominator, $1+[1+W]\beta V$. Accordingly one has the following property for W:

$$1+W(0,\beta_c)=-1/\beta_c V(0). \tag{18}$$

The manner in which the zero-wave-vector susceptibility diverges as β approaches β_c can furthermore be inferred from recent numerical analyses of high-temperature series for nearest-neighbor Ising models. It is found that[8]

$$\Psi(0,\beta)\sim\text{const}/(\beta_c-\beta)^{\gamma} \quad (\beta<\beta_c), \tag{19}$$

where $1<\gamma<2$. In view of the explicit occurrence of β in Ψ's denominator, W must have precisely the correct *linear* temperature variation at β_c+0, in order to effect a cancellation in the denominator to leading order. Since (19) is probably valid for all (ferromagnetic) interactions of sufficiently short range to permit existence of second spatial moments, one evidently has the result:

$$\partial W(0,\beta_c+0)/\partial\beta=1/\beta_c^2 V(0). \tag{20}$$

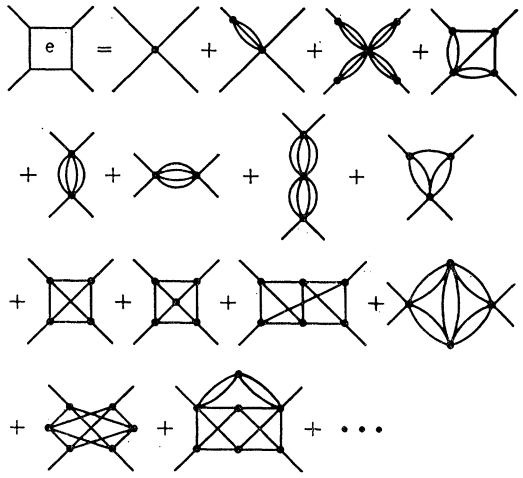

FIG. 7. Some of the low-order irreducible four-terminal diagrams contributing to the symmetric function $e(\mathbf{r}_{12},\mathbf{r}_{13},\mathbf{r}_{14})$.

The mean energy of interaction, on a per-spin basis, is obtained by summing the product $\frac{1}{2}v\psi$ over the domain of relative positions:

$$\frac{E(\beta)}{N}=\tfrac{1}{2}\sum_{\mathbf{r}_{12}} v(\mathbf{r}_{12})\psi(\mathbf{r}_{21},\beta) =\frac{1}{2\tau}\int_{\tau}\frac{[1+W(\mathbf{k},\beta)]V(\mathbf{k})}{1+[1+W(\mathbf{k},\beta)]\beta V(\mathbf{k})}d\mathbf{k}. \tag{21}$$

Differentiation with respect to β then leads to an expression for the specific heat:

$$\frac{C(\beta)}{k_B N}=-\beta^2\frac{\partial}{\partial\beta}\frac{E(\beta)}{N} =\frac{\beta^2}{2\tau}\int_{\tau}\frac{\{[1+W(\mathbf{k},\beta)]^2V(\mathbf{k})-\partial W(\mathbf{k},\beta)/\partial\beta\}V(\mathbf{k})}{\{1+[1+W(\mathbf{k},\beta)]\beta V(\mathbf{k})\}^2}d\mathbf{k}. \tag{22}$$

A more revealing form is obtained by multiplying Eq. (5) for $\mathbf{r}_{12}=0$,

$$1=\frac{1}{\tau}\int_{\tau}d\mathbf{k}\frac{1+W(\mathbf{k},\beta)}{1+[1+W(\mathbf{k},\beta)]\beta V(\mathbf{k})}, \tag{23}$$

by $\frac{1}{2}V(0)$, applying $\beta^2(\partial/\partial\beta)$ to both sides, and adding the results to Eq. (22):

$$\frac{C(\beta)}{k_B N}=\frac{\beta^2}{2\tau}\int_{\tau}d\mathbf{k}\frac{[V(\mathbf{k})-V(0)]\{[1+W(\mathbf{k},\beta)]^2V(\mathbf{k})-\partial W(\mathbf{k},\beta)/\partial\beta\}}{\{1+[1+W(\mathbf{k},\beta)]\beta V(\mathbf{k})\}^2}. \tag{24}$$

[15] For simplicity, only this case will be considered in the remainder of the paper.

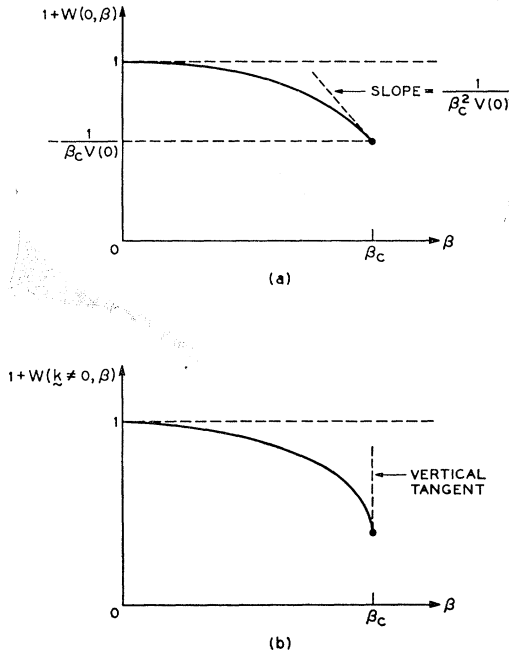

FIG. 8. Temperature dependence of $1+W(\mathbf{k},\beta)$, (a) at $\mathbf{k}=0$, (b) for some $\mathbf{k}\neq 0$ in τ.

Precisely at β_c, the denominator-factor $\mathbf{k}$ dependence near $\mathbf{k}=0$ is known to be[16]:

$$1+[1+W(\mathbf{k},\beta_c)]\beta_c V(\mathbf{k})\sim \text{const}\times k^{2-\eta} \qquad (25)$$

(aside, possibly, from unimportant angular modulation), where $\eta=\frac{1}{4}$ in two dimensions, and is approximately 0.06 in three dimensions.[17] For short-ranged potentials, $V(\mathbf{k})-V(0)$ vanishes quadratically at $\mathbf{k}=0$. When this fact is combined with the vanishing of the second numerator factor of (24) at $\mathbf{k}=0,\beta_c$ according to Eqs. (18) and (20), and the k^{d-1} (in d dimensions) from spherical-coordinate $\mathbf{k}$-space volume element $d\mathbf{k}$, one sees that Eq. (24)'s apparent singular behavior at $\mathbf{k}=0,\beta_c$ due to the denominator zero is completely quenched. In order to obtain an infinite specific heat anomaly at β_c then it is obvious that the integrand in (24) must become infinite away from $\mathbf{k}=0$, and this could only happen by $\partial W(\mathbf{k}\neq 0,\beta_c+0)/\partial\beta$ diverging to minus infinity. Figure 8 illustrates the behavior of $W(\mathbf{k},\beta)$ so far deduced.[18]

Because $V(\mathbf{k})$ is quadratic in k around the origin, whereas (25) displays "sharper" behavior (i.e., an exponent less than 2), it is clear that $W(\mathbf{k},\beta_c)$ must itself possess the $k^{2-\eta}$ sharpness. As shown in Fig. 9, the linear temperature variation of $W(0,\beta)$ at β_c, coupled with divergence of $\partial W(k\neq 0,\beta)/\partial\beta$ just deduced, is fully consistent with development of this sharpness from a smooth $W(\mathbf{k},\beta<\beta_c)$.

[16] M. E. Fisher, Physica 28, 172 (1962).
[17] M. E. Fisher, J. Math. Phys. 5, 944 (1964).
[18] It is easy to show that the leading high-temperature variation of $W(\mathbf{k},\beta)$ is a $\mathbf{k}$-independent contribution proportional to β^2.

From the defining expression for the pair correlation function,

$$\psi(\mathbf{r}_{12},\beta)=Z^{-1}(\beta)\sum_{\mu_1\ldots\mu_N=\pm 1}\mu_1\mu_2 \times\exp[-\beta\sum_{i<j=1}^{N}v(\mathbf{r}_{ij})\mu_i\mu_j], \qquad (26)$$

a temperature differential equation may be obtained by applying a β derivative to both sides:

$$\frac{\partial\psi(\mathbf{r}_{12},\beta)}{\partial\beta}=-\sum_{i<j=1}^{N}v(\mathbf{r}_{ij})\Gamma(12|ij),$$
$$\Gamma(12|ij)=\langle\mu_1\mu_2\mu_i\mu_j\rangle-\langle\mu_1\mu_2\rangle\langle\mu_i\mu_j\rangle \qquad (27)$$
$$=\psi^{(4)}(12ij)+\psi(1i)\psi(2j)+\psi(1j)\psi(2i).$$

Reference to the first form in Eq. (22) therefore gives an alternative specific heat expression in terms of $\mathbf{r}$-space functions:

$$\frac{C(\beta)}{k_BN}=-\frac{\beta^2}{2}\sum_{\mathbf{r}_{12}}v(\mathbf{r}_{12})\frac{\partial\psi(\mathbf{r}_{21},\beta)}{\partial\beta} =\frac{\beta^2}{2}\sum_{\mathbf{r}_{12},\mathbf{r}_i,\mathbf{r}_{ij}}v(\mathbf{r}_{12})v(\mathbf{r}_{ij})\Gamma(12|ij). \qquad (28)$$

The quantity $\Gamma(12|ij)$ represents the extra correlation between a pair of correlated pairs, arising when these two pairs, (12) and (ij), approach one another. The important configurations for Γ in Eq. (28) of course have these two pairs each at small separation, since v is short ranged. Γ naturally should exhibit some dependence on mutual orientation of the two pairs, but this should be relatively minor at large separations. In order that the right-hand member of Eq. (28) be able to diverge at β_c, then, it is necessary to invoke a long-range behavior for Γ as a function of R, the separation between the centers of mass of the two pairs (12) and

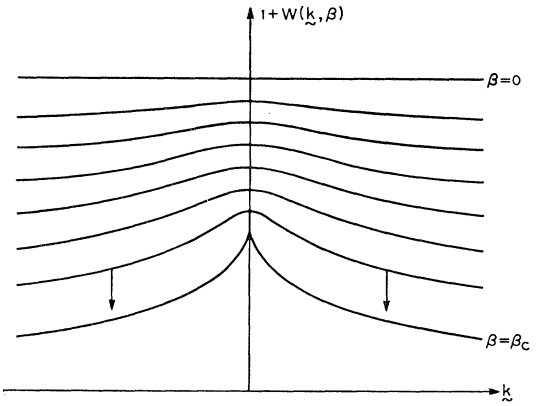

FIG. 9. Diagram showing necessity of infinitely rapid decline of "wings" of $W(\mathbf{k},\beta)$ at β_c in order to produce sharper-than-quadratic behavior at $\mathbf{k}=0$ (here highly exaggerated).

(ij). Consistent with current notions about the long-range character of the pair correlation function itself,[16,17] one would assume the following large-R asymptote:

$$\Gamma(12|ij)\sim\text{const}\times\exp(-\kappa R)/R^{\theta}, \tag{29}$$

where κ is the same exponential damping constant encountered in the pair correlation function, which may be taken proportional to $|\beta_c-\beta|^{\nu}$, $\nu>0$ in the critical region.[19]

For the purpose of singularity estimate, we may suppress pair internal degrees of freedom in Eq. (28), and replace the sum by an integral:

$$\begin{aligned}\frac{C(\beta)}{k_BN}&\sim\text{const}\times\int_1^{\infty}\frac{\exp(-\kappa R)}{R^{\theta}}R^{d-1}dR\\ &\sim\text{const}\times|\beta_c-\beta|^{\nu(\theta-d)}, \quad (\theta<d)\\ &\sim\text{const}\times\ln|\beta_c-\beta|, \quad (\theta=d).\end{aligned} \tag{30}$$

The rigorously known two-dimensional logarithmic divergence thus appears to demand $\theta=2$ (since there $\nu=1$[8]), in distinct contrast to the known pair correlation exponent $\frac{1}{4}$,[20] and this presumption is verified in the Appendix by direct calculation on the two-dimensional square net. Again in three dimensions, the specific heat is either logarithmic or characteristic of a very small negative power of $|\beta_c-\beta|$, so $\theta\approx3$ (since $\nu\approx0.65$)[17] unlike the pair correlation exponent ≈1.06.[17] One is therefore confronted with a paradox to unravel: the critical pair correlation function of pairs of spins is entirely different from that for single spins.

Finally, with use of Eqs. (5) and (12), we may Fourier transform the β variation equation for ψ, Eq. (27), and modify it into one for the β dependence of W

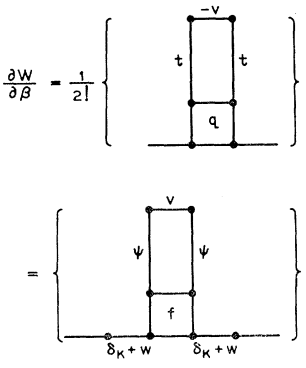

FIG. 10. Graphical version of Eq. (31). Since β only occurs in the members of the W diagram set as $-\beta v$ bonds, β differentiation provides a second pair of roots, to permit the four-terminal function $Q(q)$ to be distinguished. Symmetry factor $(2!)^{-1}$ arises from indistinguishability of the t bonds. The modified vertex function $F(f)$ is defined in Eq. (42).

[19] This identification is suggested by transfer matrix formulations for order-disorder problems, in which κ is related to the ratio of the first two eigenvalues of the characteristic matrix; see J. Ashkin and W. E. Lamb, Jr., Phys. Rev. **64**, 159 (1943).

[20] F. H. Stillinger, Jr., and H. L. Frisch, Physica **27**, 751 (1961).

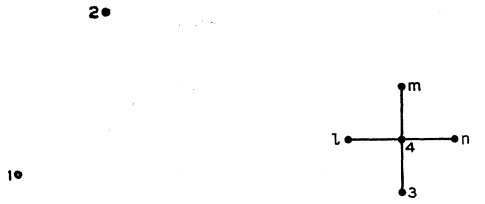

FIG. 11. Configuration of spins in a lattice of coordination number four, for which identity (41) of the text applies. Spins 3, l, m, and n are the nearest neighbors of spin 4.

explicitly in terms of Q:

$$\frac{\partial W(\mathbf{k},\beta)}{\partial\beta}=-\frac{1}{2\tau}\int_{\tau}\frac{V(\mathbf{k}')Q(\mathbf{k},\mathbf{k}',-\mathbf{k}',\beta)}{\{1+[1+W(\mathbf{k}',\beta)]\beta V(\mathbf{k}')\}^2}d\mathbf{k}'. \tag{31}$$

Figure 10 displays this equation in graphical form, showing that β differentiation of the doubly rooted W-graph set (specified in detail in Ref. 1) provides another pair of roots, and thus generates the set $\mathbf{R}$ for Q.

V. NECESSARY CONDITIONS ON Q

Because there is no general analytic procedure available for calculation of the complex e diagrams (and thence q), there is good reason for seeking restrictive conditions on functions arising in the theory that may be established independently of specific diagram evaluations. In this section we list some necessary conditions on the four-terminal function q, which are probably independent of one another.

(A) As acknowledged earlier, $q(\mathbf{r}_{12},\mathbf{r}_{13},\mathbf{r}_{14},\beta)$ must be invariant to permutation of its three independent vector variables. In addition of course q must exhibit inversion symmetry

$$q(\mathbf{r}_{12},\mathbf{r}_{13},\mathbf{r}_{14},\beta)=q(-\mathbf{r}_{12},-\mathbf{r}_{13},-\mathbf{r}_{14},\beta). \tag{32}$$

Also q will possess the same rotational symmetry (all three vectors being simultaneously rotated), and reflection symmetry as the underlying lattice.

(B) Temperature Eq. (31) permits deduction of $W(\mathbf{k},\beta)$ from a given function Q, and t and ψ follow in turn. Equations (11) and (12) then provide the quadruplet spin average, now a functional of Q, which must necessarily satisfy the inequality

$$-1\leq\langle\mu_1\mu_2\mu_3\mu_4\rangle\leq1 \tag{33}$$

for all $\mathbf{r}_{12}$, $\mathbf{r}_{13}$, $\mathbf{r}_{14}$, and β. Equality is attained in this restriction only at absolute zero, or if the four sites are identical.

(C) The coupled topological relations (15) and (17) indicate that q is a special functional of e and W (through l) which can be obtained by self-consistent solution of these two relations. In view of the nonlinearity, one can hardly expect that an arbitrary real q could have come from some real W, e pair; only a

restricted class of q's consistent with (15) and (17) is available in principle.

(D) It is obvious that if any two spins in the average $\langle\mu_1\mu_2\mu_3\mu_4\rangle$ are coincidentally the same, this quantity reduces to the pair correlation function for the remaining two spins, since always $\mu_i^2=1$. An exactly equivalent statement may be posed in terms of $\psi^{(4)}$ from Eq. (11):

$$\psi^{(4)}(\mathbf{r}_{12},\mathbf{r}_{13},\mathbf{r}_{13})=-2\psi(\mathbf{r}_{13})\psi(\mathbf{r}_{23}). \tag{34}$$

In view of Eq. (12), this may be expressed alternatively in a way explicitly containing Q,

$$\frac{1}{\tau}\int_\tau d\mathbf{k}_2 T(\mathbf{k}_2)T(-\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}_4)Q(\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4) =-2[1+W(\mathbf{k}_3)][1+W(\mathbf{k}_4)]. \tag{35}$$

(E) For lattices with coordination number four (including both two and three-dimensional cases), and just nearest-neighbor interactions $-J\mu_i\mu_j$, an additional restraint is available which follows from the Fisher identities[21,22] for these lattices. As shown in Fig. 11, let spins μ_1, μ_2, and μ_3 be located anywhere in the lattice, but take μ_4 to be a nearest neighbor to μ_3. Symbolically denote the remaining μ_4 nearest neighbors by μ_l, μ_m, and μ_n. By definition,

$$\langle\mu_1\mu_2\mu_3\mu_4\rangle=Z^{-1}(\beta)\sum_{\mu_1\cdots\mu_N=\pm1}\mu_1\mu_2\mu_3\mu_4 \times\exp(\beta J\sum_{(n.n.)}\mu_i\mu_j). \tag{36}$$

For any set of values ±1 for the four spins neighboring μ_4, we have the following identity:

$$\sum_{\mu=\pm1}\mu_4\exp[\beta J\mu_4(\mu_3+\mu_l+\mu_m+\mu_n)] =A(\beta J)(\mu_3+\mu_l+\mu_m+\mu_n) +B(\beta J)(\mu_3\mu_l\mu_m+\mu_3\mu_l\mu_n+\mu_3\mu_m\mu_n+\mu_l\mu_m\mu_n); \tag{37}$$

$$A(\beta J)=\tfrac{1}{8}[\tanh(4\beta J)+2\tanh(2\beta J)], \quad B(\beta J)=\tfrac{1}{8}[\tanh(4\beta J)-2\tanh(2\beta J)]. \tag{38}$$

If this last relation is substituted into Eq. (36), with the μ_4 sum performed first, one obtains

$$\langle\mu_1\mu_2\mu_3\mu_4\rangle=A(\beta J)[\langle\mu_1\mu_2\rangle+\langle\mu_1\mu_2\mu_3\mu_l\rangle +\langle\mu_1\mu_2\mu_3\mu_m\rangle+\langle\mu_1\mu_2\mu_3\mu_n\rangle] +B(\beta J)[\langle\mu_1\mu_2\mu_l\mu_m\rangle+\langle\mu_1\mu_2\mu_l\mu_n\rangle +\langle\mu_1\mu_2\mu_m\mu_n\rangle+\langle\mu_1\mu_2\mu_3\mu_l\mu_m\mu_n\rangle]. \tag{39}$$

The sextuplet spin average may be eliminated by use of identity (37) in an expression of type (36) for $\langle\mu_1\mu_2\mu_l\mu_4\rangle$; as a result it is verified that

$$\langle\mu_1\mu_2\mu_l\mu_4\rangle=A(\beta J)[\langle\mu_1\mu_2\mu_l\mu_3\rangle+\langle\mu_1\mu_2\rangle +\langle\mu_1\mu_2\mu_l\mu_m\rangle+\langle\mu_1\mu_2\mu_l\mu_n\rangle] +B(\beta J)[\langle\mu_1\mu_2\mu_3\mu_m\rangle+\langle\mu_1\mu_2\mu_3\mu_n\rangle +\langle\mu_1\mu_2\mu_3\mu_l\mu_m\mu_n\rangle+\langle\mu_1\mu_2\mu_m\mu_n\rangle]. \tag{40}$$

[21] M. E. Fisher, Phys. Rev. **113**, 969 (1959).
[22] F. H. Stillinger, Jr., Phys. Rev. **131**, 2027 (1963).

Finally subtract Eq. (40) from Eq. (39) to obtain the desired condition:

$$\langle\mu_1\mu_2\mu_3\mu_4\rangle-\tfrac{1}{2}\tanh(2\beta J)[\langle\mu_1\mu_2\mu_3\mu_m\rangle+\langle\mu_1\mu_2\mu_3\mu_n\rangle] =\langle\mu_1\mu_2\mu_l\mu_4\rangle-\tfrac{1}{2}\tanh(2\beta J) \times[\langle\mu_1\mu_2\mu_l\mu_m\rangle+\langle\mu_1\mu_2\mu_l\mu_n\rangle]. \tag{41}$$

Again, this limits in principle the available class of four-terminal functions q from which the quadruplet spin averages in (41) may be obtained.

VI. SELF-CONSISTENT APPROXIMATION FOR q

We turn now to use of some of the necessary conditions listed in the previous Section for development of a self-consistent approximation scheme for the four-point function Q. First, rewrite Eq. (35) in the somewhat simpler form:

$$1=\frac{1}{\tau}\int_\tau d\mathbf{k}_2\,\Psi(\mathbf{k}_2,\beta)\Psi(-\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}_4,\beta)F(\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4,\beta),$$

$$Q(\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4,\beta) =-2[1+W(\mathbf{k}_2,\beta)][1+W(\mathbf{k}_3,\beta)][1+W(\mathbf{k}_4,\beta)] \times[1+W(-\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}_4,\beta)]F(\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4,\beta). \tag{42}$$

The $\mathbf{r}$-space equivalent form of (42) is:

$$\delta_K(\mathbf{r}_{15})\delta_K(\mathbf{r}_{25})=\sum_{\mathbf{r}_3,\mathbf{r}_4}f(\mathbf{r}_{12},\mathbf{r}_{13},\mathbf{r}_{14})\psi(\mathbf{r}_{35},\beta)\psi(\mathbf{r}_{45},\beta), \tag{43}$$

where $\delta_K(\mathbf{r})$ is the lattice Kronecker delta function.

Because Eq. (43) is true for each set of vectors $\mathbf{r}_{15}$, $\mathbf{r}_{25}$, it is capable, so to say, of entirely determining a function of two vector variables. Therefore if the symmetric function f had the following form, for example[23]:

$$f(\mathbf{r}_{12},\mathbf{r}_{13},\mathbf{r}_{14})=\chi(\mathbf{r}_{13},\mathbf{r}_{14})\delta_K(\mathbf{r}_{12}) +\chi(\mathbf{r}_{12},\mathbf{r}_{14})\delta_K(\mathbf{r}_{13})+\chi(\mathbf{r}_{12},\mathbf{r}_{13})\delta_K(\mathbf{r}_{14}) +\chi(\mathbf{r}_{21},\mathbf{r}_{24})\delta_K(\mathbf{r}_{23})+\chi(\mathbf{r}_{21},\mathbf{r}_{23})\delta_K(\mathbf{r}_{24}) +\chi(\mathbf{r}_{31},\mathbf{r}_{32})\delta_K(\mathbf{r}_{34}), \tag{44}$$

with χ symmetric in its two variables, then (43) would completely determine χ, and a closed Ising model theory would result. Of course (44) doubtless represents an approximation to the correct f, but the attractive notion of contracting the function f onto a symmetric combination of functions of fewer variables, with consequently a means for evaluating f, comprises the basic theme in the remainder of this article.

Actually we shall investigate a more severe contraction than shown in Eq. (44). Let[23]

$$f(\mathbf{r}_{12},\mathbf{r}_{13},\mathbf{r}_{14})\cong\varphi(\mathbf{r}_{13})\delta_K(\mathbf{r}_{12})\delta_K(\mathbf{r}_{34}) +\varphi(\mathbf{r}_{12})\delta_K(\mathbf{r}_{13})\delta_K(\mathbf{r}_{24})+\varphi(\mathbf{r}_{12})\delta_K(\mathbf{r}_{14})\delta_K(\mathbf{r}_{23}). \tag{45}$$

[23] The compression of f onto subspaces for coincidence of two or more of the four terminals is analogous to the introduction of pseudopotentials in scattering theory.

If this approximation for f is adopted, the restraint condition (43) could not generally be satisfied for all $\mathbf{r}_{15}$, $\mathbf{r}_{25}$. However we can demand that it be satisfied on the $\mathbf{r}_{12}=0$ subspace, and in doing so get a determining equation for φ:

$$\delta_K(\mathbf{r}_{15})=\sum_{\mathbf{r}_3}\varphi(\mathbf{r}_{13})\psi^2(\mathbf{r}_{35})+2\varphi(0)\psi^2(\mathbf{r}_{15}). \quad (46)$$

This linear sum equation may readily be solved by taking Fourier transforms. If

$$[\Phi(\mathbf{k}),\Psi^{(2)}(\mathbf{k})]=\sum_{\mathbf{r}}[\varphi(\mathbf{r}),\psi^2(\mathbf{r})]\exp(i\mathbf{k}\cdot\mathbf{r}), \quad (47)$$

the transformed version of Eq. (46) is

$$1=\Phi(\mathbf{k})\Psi^{(2)}(\mathbf{k})+2\varphi(0)\Psi^{(2)}(\mathbf{k}) \quad (48)$$

or

$$\Phi(\mathbf{k})=[\Psi^{(2)}(\mathbf{k})]^{-1}-2\varphi(0). \quad (49)$$

The inverse transform next yields an expression for $\varphi(\mathbf{r})$:

$$\varphi(\mathbf{r},\beta)=\frac{1}{\tau}\int_\tau d\mathbf{k}\frac{\exp(-i\mathbf{k}\cdot\mathbf{r})-\frac{2}{3}\delta_K(\mathbf{r})}{\Psi^{(2)}(\mathbf{k},\beta)}. \quad (50)$$

With φ now in the form of an explicit functional of ψ in Eq. (50), Q in the basic β equation (31) likewise this latter equation could be then integrated to give $W(\mathbf{k},\beta)$. However it is well to recognize that the resulting approximation to W would not necessarily satisfy the sum rule Eq. (23). It is therefore advisable from the outset to split W into two parts:

$$W(\mathbf{k},\beta)=W_0(\beta)+W_1(\mathbf{k},\beta),$$
$$0=\int_\tau d\mathbf{k}W_1(\mathbf{k},\beta), \quad (51)$$

where the $\mathbf{k}$-independent W_0 is the average of W over τ, and W_1 the fluctuation about the average. Then we need use φ in temperature equation (31) only to determine the fluctuation quantity W_1, since Eq. (23) can always be used to fix W_0 at any β.

The foregoing reason therefore justifies addition of any $\mathbf{k}$-independent function of β to the right member of Eq. (31) to bring it into accord with sum rule (23). Primary interest here centers around critical phenomena becomes an explicit functional of W, and in principle above the transition temperature ($\beta\leq\beta_c$), and in view of conditions (18) and (20), insertion of Eq. (45) into Eq. (31) yields the following differential equation:

$$[\partial W(\mathbf{k},\beta)/\partial\beta]=[1/\beta_c^2V(0)]+[\partial\tilde{W}(\beta)/\partial\beta]+[1+W(\mathbf{k},\beta)]^2\left\{\frac{1}{\tau}\int_\tau d\mathbf{k}'V(\mathbf{k}')\Psi^2(\mathbf{k}')[\Phi(0)+2\Phi(\mathbf{k}-\mathbf{k}')]\right\}$$
$$-[1+W(0,\beta)]^2\left\{\frac{1}{\tau}\int_\tau d\mathbf{k}'V(\mathbf{k}')\Psi^2(\mathbf{k}')[\Phi(0)+2\Phi(-\mathbf{k}')]\right\}. \quad (52)$$

The last two terms cancel at $\mathbf{k}=0$, and the first terms would provide the correct $\mathbf{k}=0,\beta=\beta_c$ derivative by Eq. (20); in principle, then, $\tilde{W}(\beta)$ should vanish more rapidly with $\beta_c-\beta$ than the first power, in accord with Eq. (19). Equation (52) is the basic relation of the present self-consistent approximation.

It is our object to use Eq. (52) to deduce characteristic critical region exponents for thermodynamic functions as well as for correlation functions themselves. We shall see that these exponents follow uniquely from the requirements of self-consistency. The form of the pair correlation function, for example, with which we will work, is appropriate to the large-$\mathbf{r}$ limit, when β is only slightly less than β_c[16,24]:

$$\psi(\mathbf{r},\beta)\sim\exp(-\kappa r)/r^{d-2+\eta}, \quad (53)$$

where the small positive quantity η represents deviation from "classical" critical point behavior, and the exponential decay parameter has already been encountered in Eq. (29), with

$$\kappa(\beta)\sim(\beta_c-\beta)^\nu, \quad \nu>0. \quad (54)$$

The Fourier transform belonging to Eq. (53), and valid for small k, has the following form[17]:

$$\Psi(\mathbf{k},\beta)\sim(k^2+\kappa^2)^{\eta/2-1}. \quad (55)$$

The general "rule of thumb" applicable here is that the undamped asymptotic function $r^{2-d-\eta}$ transforms[25] to a function whose lowest noneven-integer power is $k^{\eta-2}$, and that damping factor $\exp(-\kappa r)$ modifies argument k to $(k^2+\kappa^2)^{1/2}$ on account of the effective upper integral cutoff at $r\approx\kappa^{-1}$.

Since $V(\mathbf{k})$ possesses a series expansion about $\mathbf{k}=0$ with leading terms quadratic in $\mathbf{k}$ components, reference to Eq. (5) shows that the critical region Ψ behavior in Eq. (55), assuming $\eta>0$, could only result from a $W(\mathbf{k},\beta)$ which itself bore the nonintegral exponent:

$$1+W(\mathbf{k},\beta)\sim 1+W(0,\beta_c)+[\beta/\beta_c^2V(0)]-(k^2+\kappa^2)^{1-\eta/2}, \quad (56)$$

[24] Both multiplicative constants and angular modulations of order unity will be suppressed in the asymptotes quoted in this section for the sake of brevity. They are irrelevant for the argument determining exponents.

[25] R. J. Duffin, Duke Math. J. 20, 233 (1953).

the third term having been included on account of Eq. (20). Hence the small-$\mathbf{k}$ behavior of the important Ψ denominator is obtained by use of (56) and the binomial expansion:

$$1+[1+W(\mathbf{k},\beta)]\beta V(\mathbf{k})\sim\kappa^{2-\eta}+\kappa^{-\eta}k^2+\cdots, \quad (57)$$

with neglect of $O(k^4)$ terms. The leading term in this last expression is the $\tilde{W}(\beta)$ contribution, which therefore varies as $(\beta_c-\beta)^{\nu(2-\eta)}$. The zero-wave-vector susceptibility $\Psi(0,\beta)$ then varies as $(\beta_c-\beta)^{\nu(\eta-2)}$, which identifies the exponent γ introduced in Eq. (19),

$$\gamma=\nu(2-\eta). \quad (58)$$

By squaring the asymptote shown in Eq. (53), we may next conclude that the transform $\Psi^{(2)}$ occurring in our φ expression (50) has the following small-$\mathbf{k}$ behavior:

$$\Psi^{(2)}(\mathbf{k},\beta)\sim(k^2+\kappa^2)^{d/2-2+\eta}, \quad (59)$$

presuming that η is small enough that the exponent is still negative. Therefore,

$$\Phi(\mathbf{k},\beta)\sim\Phi(0,\beta_c)+(k^2+\kappa^2)^{2-d/2-\eta}, \quad (60)$$

which would have been the result of transforming:

$$\varphi(\mathbf{r},\beta)\sim\exp(-\kappa r)/r^{d-2+\eta}. \quad (61)$$

A key point to establish is the $\mathbf{k}$ variation of the convolution integral occurring in the temperature equation (52),

$$\frac{1}{\tau}\int_\tau d\mathbf{k}'V(\mathbf{k}')\Psi^2(\mathbf{k}',\beta)\Phi(\mathbf{k}-\mathbf{k}',\beta). \quad (62)$$

Again it is the small-$\mathbf{k}'$ values that are of importance in the integrand, and for them, V may simply be reckoned as a negative constant, leaving a convolution of Ψ^2 and Φ. The Fourier theorem then permits (62) to be written as a lattice sum involving the product of functions whose transforms are Ψ^2 and Φ, respectively, so one estimates for (62):

$$-\sum_{\mathbf{r}}\exp(i\mathbf{k}\cdot\mathbf{r})\frac{\exp(-\kappa r)}{r^{d-4+2\eta}}\frac{\exp(-\kappa r)}{r^{4-2\eta}}\sim-\ln(k^2+\kappa^2). \quad (63)$$

We wish now to match up exponents of $(\beta_c-\beta)$, by comparing coefficient of k^2 on both sides of temperature equation (52). For the left member, use expression (56); the dominant contribution to the right member clearly is the coefficient of k^2 in small-$\mathbf{k}$ expansion of estimate (63). Therefore one finds that $(\partial/\partial\beta)(-\kappa^{-\eta}k^2)$ and $-\kappa^{-2}k^2$ must be comparable quantities, i.e.,

$$(\beta_c-\beta)^{-\nu\eta-1}=(\beta_c-\beta)^{-2\nu}, \qquad \eta=2-(1/\nu). \quad (64)$$

By referring to Eq. (58), it is clear that the present approximation has the Curie-Weiss susceptibility law ($\gamma=1$) as a logical consequence. For that reason, the approximation is not capable of honoring the condition set down in Eq. (20), and $\tilde{W}$ will vary linearly with $\beta_c-\beta$ at β_c.

The next step is to integrate differential equation (52) with respect to β at a given (small) value of k. For a chosen k value, the last two terms of (52) cancel one another to within a difference of order unity until β exceeds $\beta_c-k^{1/\nu}$; when β exceeds $\beta_c-k^{1/\nu}$ on the other hand they yield essentially $-\ln(1+k^2/\kappa^2)$ [on account of (63)], which for present purposes is equivalent to $-\ln(k^2/\kappa^2)$. We therefore calculate $W(\mathbf{k},\beta)$ to be equal to a function well behaved in both k and β *plus* a singular contribution of the type:

$$-\int_{\beta_c-k^{1/\nu}}^{\beta}d\beta'\ln\left[\frac{k^2}{(\beta_c-\beta')^{2\nu}}\right] =2\nu[\beta_c-\beta-k^{1/\nu}]+(\beta_c-\beta)\ln\frac{k^2}{\kappa^2}, \quad (65)$$

assuming that the upper integration limit exceeds the lower limit. Since Eq. (64) states that $1/\nu=2-\eta$, it is clear that the first term on the right in Eq. (65) yields the β_c profile sharper at the origin than parabolic. For k smaller than $(\beta_c-\beta)^\nu$, on the other hand, (65) becomes modified in the manner qualitatively indicated in (56) by the use of argument $(k^2+\kappa^2)^{1/2}$ in place of k, so that W remains "rounded" at $\mathbf{k}=0$ when $\beta<\beta_c$.

The last term in (65) is a key result. It states that for any $\mathbf{k}$ away from the origin, a β sufficiently close to β_c is eventually reached such that $W(\mathbf{k},\beta)$ varies with temperature in the manner of a constant plus $(\beta-\beta_c)\ln(\beta_c-\beta)$. Specific heat expression (24) thereupon leads inevitably to the conclusion that $C(\beta)$ possesses an infinite anomaly of logarithmic character as β approaches β_c from below (the disordered phase).

The remaining relation between exponents required to fix them uniquely follows from sum rule (23). Note that as β approaches β_c from below, variation of both numerator and denominator W's in Eq. (23) for large $\mathbf{k}$ tends to reduce the value of the integral by contributions of the type $-(\beta_c-\beta)\ln(\beta_c-\beta)$. The only way that the required constancy of the integral can be insured is by having an equivalent increasing contribution from the denominator (which is developing a zero at $\mathbf{k}=0$) for k's less than or equal to about κ. In view of Eq. (57), this latter may be estimated by means of the following integral:

$$\int_0^\kappa\left[\frac{1}{k^{2-\eta}}-\frac{1}{\kappa^{2-\eta}}\right]k^{d-1}dk\approx(\beta_c-\beta)^{\nu(d-2+\eta)}. \quad (66)$$

This estimate need be taken seriously only so far as the exponent of $(\beta_c-\beta)$ is concerned, and could in fact have been multiplied by any function of $\beta_c-\beta$ (such as the logarithm) which is dominated by any negative power of this variable at the origin. Consequently, we must demand that

$$\nu(d-2+\eta)=1. \quad (67)$$

Because of relation (64), we conclude that the self-consistent solution implied by functional assumption (45) requires:

$$\eta=2-(d/2), \tag{68}$$

and

$$\nu=2/d. \tag{69}$$

Although the estimate of η is probably too high, it is interesting to note that the ν prediction is apparently exact in two dimensions (at least for nearest-neighbor interactions), and in good agreement with the numerical result (0.644 ± 0.003) obtained by Fisher and Burford in three dimensions.[17]

Of course in one dimension with short-range interactions no phase transition is expected, so the above analysis does not apply. In four or more dimensions, the self-consistent solution does not differ (so far as critical exponents are concerned) from the corresponding spherical model approximation, since $W(\mathbf{k},\beta_c)$ is no longer "sharper" at $\mathbf{k}=0$ than $V(\mathbf{k})$, and thus $\eta=0$ and $\nu=(d-2)^{-1}$.

For $\beta>\beta_c$, approximation (45) is entirely inadequate to deal with the long-range order that the system should possess, leading in fact to spurious divergences. The reason is evident from the second form of the graphical equation shown in Fig. 10. In the presence of long-range order, the pair correlation function will possess a long-range constant part equal to the square of the magnetization $m(\beta)$, plus a short-range part ψ_s:

$$\psi(\mathbf{r},\beta)=\psi_s(\mathbf{r},\beta)+m^2(\beta) \quad (\beta>\beta_c). \tag{70}$$

Remembering that $v(\mathbf{r})$ is short ranged, it is clear that summation over the uppermost pair of vertices in the diagram will give a result proportional to N, rather than of order unity as was the case when $\beta<\beta_c$. The weakened version (46) of more general condition (43) induces cancellation of these order N contributions only when the bottom pair of the four f terminals are coincident, but leaves them uncompensated when the terminal pair is distinct. Only by use of the complete condition (43) can a proper theory be constructed which extends through β_c, with prediction of the magnetization curve $m(\beta)$. This of course would require returning to the less stringent approximation for f in Eq. (44); the full condition (43) then leads to a linear integral equation for X, the Fourier transform of χ:

$$X(\mathbf{k}_3,\mathbf{k}_4)=\left[\frac{1}{\tau}\int_\tau d\mathbf{k}_2\Psi(\mathbf{k}_1)\Psi(\mathbf{k}_2)\right]^{-1}$$
$$\times\left\{1-\frac{1}{\tau}\int_\tau d\mathbf{k}_2\Psi(\mathbf{k}_1)\Psi(\mathbf{k}_2)[X(\mathbf{k}_1,\mathbf{k}_2)\right.$$
$$+X(\mathbf{k}_1,\mathbf{k}_3)+X(\mathbf{k}_1,\mathbf{k}_4)+X(\mathbf{k}_2,\mathbf{k}_3)$$
$$\left.+X(\mathbf{k}_2,\mathbf{k}_4)]\right\}, \tag{71}$$

$$X(\mathbf{k}_3,\mathbf{k}_4)=\sum_{r_3,r_4}\exp[i(\mathbf{k}_3\cdot\mathbf{r}_{13}+\mathbf{k}_4\cdot\mathbf{r}_{14}]\chi(\mathbf{r}_{13},\mathbf{r}_{14}),$$

$$\mathbf{k}_1=-\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}_4,$$

whose solution for X as a functional of Ψ then would serve as starting point for an improved theory.

VII. FINAL COMMENTS

The $k^{-d/2}$ wavelength-dependent critical susceptibility, the logarithmic specific heat singularity, and the Curie-Weiss behavior for the $\mathbf{k}=0$ susceptibility are all contained within the Patashinskii-Pokrovskii[12] transition theory for He^4, as well as within Abe's[4] transcription to the Ising model transition. The underlying structure of the present approximate theory however is somewhat different, and can be argued to possess a more satisfactory logical basis. In particular, close attention has been paid to sum rule (23), with the result that the specific heat anomaly arises from large-$\mathbf{k}$ values of the boson "excitation spectrum" rather than from small $\mathbf{k}$, i.e., from pair correlation at small distance, rather than large distance, as must certainly be the case with short-ranged $v(\mathbf{r})$. In addition, it is clear in the present analysis that $W(\mathbf{k},\beta)$ is singular at $\mathbf{k}=0$ *only* when $\beta=\beta_c$, whereas the analogous quantities in Refs. 4 and 12 retain their singular $\mathbf{k}=0$ behavior throughout the critical region. Finally, the Curie-Weiss value of unity for γ follows as a logical deduction in the present context, rather than having been inserted as an additional hypothesis.

In the high-temperature regime, it is of interest to note that the approximate form for f given in Eq. (45) is asymptotically valid when only the simple diagrams of the type shown as the first three examples in Fig. 4 are of any importance. As β increases, though, diagrams of the fourth type in Fig. 4 will increase in importance, and would create deviations from the assumed form (45). Interestingly enough, the less restrictive assumption (44) is still consistent with the fourth diagram (but not the fifth), and since orders may be assigned as β raised to a power equal to the number of internal bonds, a theory based on (44) and the integral Eq. (71) would be rigorously correct to a higher order in β than the one considered at length in the previous section.

Although even extended assumption (44) for f will commit error in some order of β, this should not imply that the description of behavior of the model in the critical region is poor. On the contrary, the important part of the spectrum is clearly at small $\mathbf{k}$ in the critical region, and any approximation on the basic scattering amplitude Q which preserves its behavior for small $\mathbf{k}$'s should give a qualitatively correct account of the phenomena. The pseudopotential analogy has already been noted[23] for the subspace compression on f embodied in Eq. (44). But is is precisely the small-$\mathbf{k}$ scattering amplitude that a pseudopotential is designed to reproduce correctly.[26] It should eventually be instructive to see how critical exponents predicted on the

[26] J. M. Blatt and V. F. Weisskopf, *Theoretical Nuclear Physics* (John Wiley & Sons, Inc., New York, 1952), p. 74.

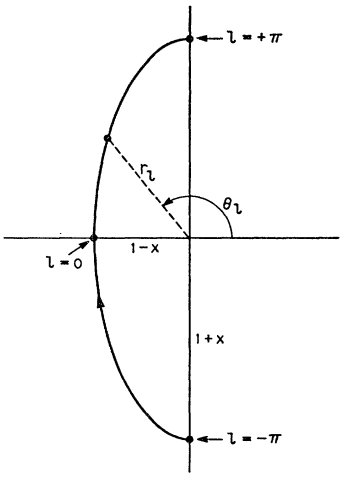

FIG. 12. Polar plot of $r_l \exp(i\theta_l)$, defined in Eq. (A10). The direction indicated on the elliptic arc is for increasing l.

basis of integral equation (71) compare with those obtained in the previous section, and those known or conjectured to be exact.[8] A favorable comparison would lend additional credence to the approach to understanding of critical phenomena through diagrammatic methods, pioneered by Green[27] in his critique of the Ornstein-Zernike hypothesis.

APPENDIX

We wish now to ascertain the result obtained for exponent θ in Eq. (29), by explicit calculation in the two-dimensional Ising model, with nearest-neighbor interaction J. Here it proves especially convenient to follow the formalism and notation introduced by Schultz, Mattis, and Lieb,[28] to whose lucid expository account the reader is referred for definition and supporting detail.

In particular, we examine just the case of four spins along the same row of the lattice, forming two nearest-neighbor pairs. Let the spins be numbered m, $m+1$, m', $m'+1$ with $m'>m+1$. Then it is required to compute

$$\langle \mu_m \mu_{m+1} \mu_{m'} \mu_{m'+1} \rangle = \lim_{M\to\infty} \langle \Psi_0^+ | \sigma_m^x \sigma_{m+1}^x \sigma_{m'}^x \sigma_{m'+1}^x | \Psi_0^+ \rangle, \quad \text{(A1)}$$

in which M is the lattice width (the row contains M spins), σ_j^x is a Pauli operator for site j, and $|\Psi_0^+\rangle$ is the relevant "vacuum" state. Although the separate-site Pauli operators do not constitute a canonical set for the problem since they satisfy mixed commutation relations, Schultz, Mattis, and Lieb show that the Jordan-Wigner transformation may be employed to introduce proper fermion operators $\mathbf{C}$, in terms of which:

$$\sigma_m^x \sigma_{m+1}^x \sigma_{m'}^x \sigma_{m'+1}^x = (i\mathbf{C}_m^y)(\mathbf{C}_{m+1}^x)(i\mathbf{C}_{m'}^y)(\mathbf{C}_{m'+1}^x). \quad \text{(A2)}$$

[27] M. S. Green, J. Chem. Phys. 33, 1403 (1960).
[28] T. D. Schultz, D. C. Mattis, and E. H. Lieb, Rev. Mod. Phys. 36, 856 (1964).

After inserting (A2) into (A1), one has only two nonvanishing contractions under operation of Wick's theorem:

$$\langle \mu_m \mu_{m+1} \mu_{m'} \mu_{m'+1} \rangle = \langle \Psi_0^+ | i\mathbf{C}_m^y \mathbf{C}_{m+1}^x | \Psi_0^+ \rangle \langle \Psi_0^+ | i\mathbf{C}_{m'}^y \mathbf{C}_{m'+1}^x | \Psi_0^+ \rangle - \langle \Psi_0^+ | i\mathbf{C}_m^y \mathbf{C}_{m'+1}^x | \Psi_0^+ \rangle \langle \Psi_0^+ | i\mathbf{C}_{m'}^y \mathbf{C}_{m+1}^x | \Psi_0^+ \rangle. \quad \text{(A3)}$$

The first term's factors may be identified as precisely those encountered in calculation of the nearest-neighbor pair correlation function for the model, and therefore give $\langle \mu_m \mu_{m+1} \rangle \langle \mu_{m'} \mu_{m'+1} \rangle$. Thus

$$\begin{aligned} \Gamma(m, m+1 | m', m'+1) &= \langle \mu_m \mu_{m+1} \mu_{m'} \mu_{m'+1} \rangle - \langle \mu_m \mu_{m+1} \rangle \langle \mu_{m'} \mu_{m'+1} \rangle \\ &= -\langle \Psi_0^+ | i\mathbf{C}_m^y \mathbf{C}_{m'+1}^x | \Psi_0^+ \rangle \langle \Psi_0^+ | i\mathbf{C}_{m'}^y \mathbf{C}_{m+1}^x | \Psi_0^+ \rangle \\ &= -a_{m,m'} a_{m',m}. \end{aligned} \quad \text{(A4)}$$

The matrix elements $a_{m,m'} = a_{m'-m}$ are shown in Ref. 28 to have a Fourier-transform structure:

$$a_{m,m'} = M^{-1} \sum_l \exp[-il(m'-m)] \times \exp[-i(2\varphi_l + l)]; \quad \text{(A5)}$$

assuming for convenience that M is even, the values of l included in the sum are

$$l = \pm\frac{\pi}{M}, \ \pm\frac{3\pi}{M}, \ \pm\frac{5\pi}{M}, \ \cdots, \ \pm\frac{(M-1)\pi}{M}. \quad \text{(A6)}$$

The set of numbers φ_l are defined at the critical temperature by the transcendental relation:

$$\exp(-4i\varphi_l) = \frac{[\exp(il)-x][\exp(il)-1]}{[\exp(-il)-x][\exp(-il)-1]}, \quad \text{(A7)}$$

to which must be appended the condition that the algebraic sign of the real number φ_l be the same as that of l:

$$\operatorname{sgn}\varphi_l = \operatorname{sgn} l. \quad \text{(A8)}$$

The parameter x in (A7) is defined:

$$\begin{aligned} x &= \coth K_c \coth K_c^*; \\ \tanh K_c^* &= \exp(-2K_c), \\ K_c &= \beta_c J. \end{aligned} \quad \text{(A9)}$$

Clearly $x>1$.

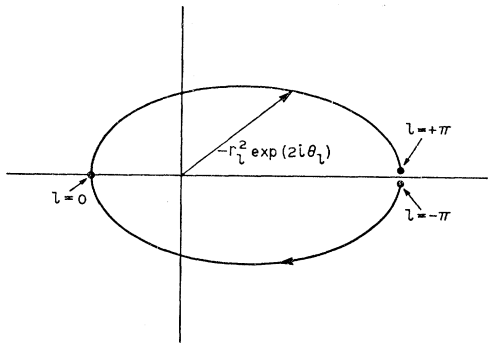

FIG. 13. Polar plot of $-r_l^2 \exp(2i\theta_l)$.

Let the real numbers r_l and θ_l be defined by:

$$r_l \exp(i\theta_l) = \exp(il/2) - x\exp(-il/2)$$
$$= (1-x)\cos(l/2) + i(1+x)\sin(l/2). \quad \text{(A10)}$$

Then Eq. (A7) is just:

$$\{\exp[-i(2\varphi_l + l)]\}^2 = -\exp(2i\theta_l). \quad \text{(A11)}$$

In the large-M limit, one sees from (A6) that the l values uniformly and densely populate the interval $-\pi < l < +\pi$. θ_l may then be read off of a polar plot of the elliptic arc defined parametrically by the last member in (A10), as shown in Fig. 12. From the figure it is clear that as l ranges from $-\pi$ to $+\pi$, θ_l decreases from $3\pi/2$ to $\pi/2$, and so $2\theta_l$ may be regarded as going from $+\pi$ down to $-\pi$. Figure 13 illustrates how $-r_l^2 \exp(2i\theta_l)$ then must vary, also on an elliptic polar plot: the polar angle decreases from 2π to 0.

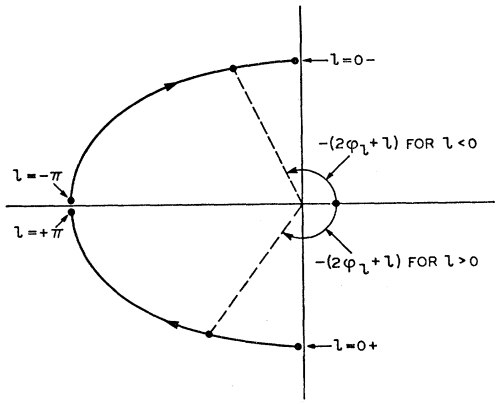

FIG. 14. Polar plot derived by taking the appropriate square root in Eq. (A11). The polar angle, $-(2\varphi_l+l)$, decreases from $+\pi$ to $+\pi/2$ as l increases from $-\pi$ to 0−, jumps discontinuously to $-\pi/2$ for $l=0+$, then decreases to $-\pi$ as l increases to $+\pi$.

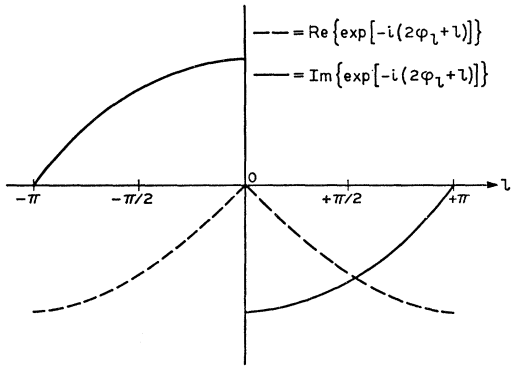

FIG. 15. Real and imaginary parts of $\exp[-i(2\varphi_l+l)]$. These functions are, respectively, even and odd in l.

We must next specify which square root to take in Eq. (A11) to find $\exp[-i(2\varphi_l+l)]$, to ensure compliance with condition (A8). One readily verifies the necessity of taking the positive root for $l<0$, and the negative root for $l>0$. Figure 14 shows the corresponding polar plot, whose polar angle for given l is $-(2\varphi_l+l)$ and which displays a sudden jump from $+\pi/2$ to $-\pi/2$ as l passes through 0.

The final Fig. 15 displays the real and imaginary parts of $\exp[-i(2\varphi_l+l)]$. The behavior of $a_{m,m'}$ for large $m'-m$ will be determined solely by the imaginary part, because it alone has a jump discontinuity at the origin. Hence

$$a_{m,m} \sim (m'-m)^{-1}$$

aside from a positive proportionality constant. Finally, then, $\Gamma(m, m+1 | m', m'+1)$ in Eq. (A4) behaves asymptotically as $(m'-m)^{-2}$ with positive proportionality constant, in agreement with the conclusion in Sec. IV.