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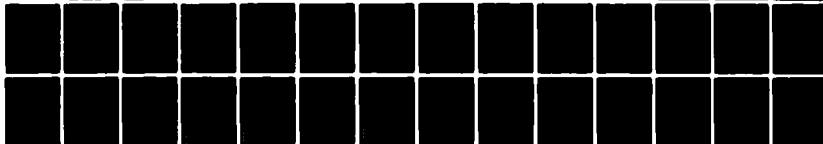
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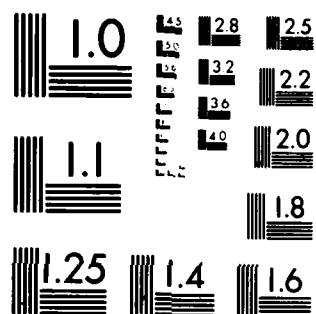
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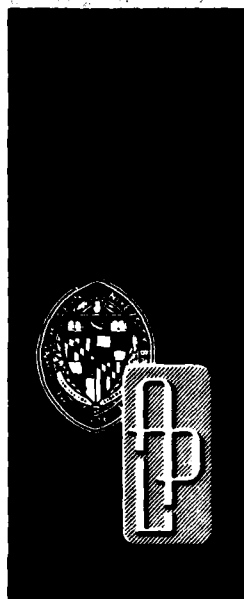
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Technical Memorandum

**DIAGRAMS FOR THE FREE ENERGY
AND DENSITY WEIGHT FACTORS OF
THE ISING MODELS**

R. A. FARRELL and S. FAVIN

The Johns Hopkins University Applied Physics Laboratory

P. H. E. MEIJER and P. ESFANDIARI

The Catholic University of America

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REPORT DOCUMENTATION PAGE	
1. REPORT NUMBER JHU/APL TG 1337	2. GOVT ACCESSION NO. AD-A226 293
4. TITLE (and Subtitle) DIAGRAMS FOR THE FREE ENERGY AND DENSITY WEIGHT FACTORS OF THE ISING MODELS	3. RECIPIENT'S CATALOG NUMBER
	5. TYPE OF REPORT & PERIOD COVERED Technical Memorandum
7. AUTHOR (s) R. A. Ferrell, S. Favin, P. H. E. Meijer, and P. Esfandiari	6. PERFORMING ORG. REPORT NUMBER TG 1337
	8. CONTRACT OR GRANT NUMBER (s) N00024-83-C-5301 N00014-78-C-0518
9. PERFORMING ORGANIZATION NAME & ADDRESS The Johns Hopkins University Applied Physics Laboratory Johns Hopkins Road Laurel, MD 20707	10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS X83J/RTP
11. CONTROLLING OFFICE NAME & ADDRESS Naval Sea Systems Command Washington, D.C. 20362	12. REPORT DATE January 1983
	13. NUMBER OF PAGES 42
14. MONITORING AGENCY NAME & ADDRESS Naval Plant Representative Office Johns Hopkins Road Laurel, MD 20707	15. SECURITY CLASS. (of this report) Unclassified
	15a. DECLASSIFICATION/DOWNGRADING SCHEDULE
16. DISTRIBUTION STATEMENT (of this Report) Approved for public release; distribution unlimited.	
17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)	
18. SUPPLEMENTARY NOTES	
19. KEY WORDS (Continue on reverse side if necessary and identify by block number) diagrammatic expansion phase transitions Ising models statistical mechanics	
20. ABSTRACT (Continue on reverse side if necessary and identify by block number) This report describes the evaluation of the free energy of the nearest neighbor Ising model through tenth order in the inverse temperature variable (J/kT). The free energy is expressed in terms of diagrams composed of interaction bonds and vertices. An explicit list of the diagrams with 10 or fewer bonds is presented, and the unrestricted lattice constants (free multiplicities) of these diagrams are given for the cubic lattices. We employ a theorem that states that a certain sum of diagrams is zero in order to obtain the density-dependent weight factors associated with the vertices. These factors are polynomials in the density and depend on the kind of articulated vertex under consideration. Explicit denumeration of the diagrams is given for those articulated vertices of the fourth and fifth kind that are needed in the tenth order expansion. These methods reproduce the known results for the cubic lattices.	

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The work described in this report was performed under U.S. Navy contracts N00024-83-C-5301 (The Johns Hopkins University Applied Physics Laboratory) and N00014-78-C-0518 (The Catholic University).

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Johns Hopkins Road, Laurel, Maryland 20707

Operating under Contract N00024-83-C-5301 with the Department of the Navy

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This report describes the evaluation of the free energy of the nearest neighbor Ising model through tenth order in the inverse temperature variable (J/kT). The free energy is expressed in terms of diagrams composed of interaction bonds and vertices. An explicit list of the diagrams with 10 or fewer bonds is presented, and the unrestricted lattice constants (free multiplicities) of these diagrams are given for the cubic lattices. We employ a theorem that states that a certain sum of diagrams is zero in order to obtain the density-dependent weight factors associated with the vertices. These factors are polynomials in the density and depend on the kind of articulated vertex under consideration. Explicit denumeration of the diagrams is given for those articulated vertices of the fourth and fifth kind that are needed in the tenth order expansion. These methods reproduce the known results for the cubic lattices.

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1. INTRODUCTION

The exact solution to the free energy of the three-dimensional Ising model is not known, but exact series expansions have proven quite beneficial for deducing the thermodynamic properties of these systems.¹⁻⁶ The terms in these series are evaluated through some order in an expansion variable, and diagrammatic methods are a valuable aid for cataloging the various contributions. The steps involved in obtaining such expansions are: (1) list the topologically distinct diagrams, (2) generate the weight factors that are associated with the vertices of the diagram, and (3) calculate the appropriate lattice

constant (the number of ways the diagram can be embedded in the lattice). The degree of difficulty of these steps, as well as the need to make modifications appropriate to the particular model (e.g., particular lattice or particular interaction potential), depend on the specific diagrammatic expansion. The present report uses an especially convenient expansion to analyze nearest-neighbor models on cubic lattices; application to other systems can be achieved by calculating the unrestricted lattice constants (i.e., free multiplicities) for them.

¹ *Phase Transitions and Critical Phenomena* Vol. 3, C. Domb and M. S. Green (eds.), Academic Press, London (1974).

² M. F. Sykes, D. S. Gaunt, P. D. Roberts, and J. A. Wyles, "High Temperature Series for the Susceptibility of the Ising Model; I. Two Dimensional Lattices, and II. Three Dimensional Lattices," *J. Phys. A* **5**, 6, 640 (1972).

³ M. F. Sykes, D. L. Hunter, D. S. McKenzie, and B. R. Heap, "Specific Heat of a Three Dimensional Ising Ferromagnet above the Curie Temperature T_C ," *J. Phys. A* **5**, 667 (1972).

⁴ P. H. E. Meijer and R. A. Farrell, "Padé Approximations and the Critical Exponents in the Two- and Three-Dimensional Ising Models," *Phys. Rev. B* **12**, 3 (1975).

⁵ D. S. Gaunt and G. A. Baker, Jr., "Low-temperature Critical Exponents from High-temperature Series: The Ising Model," *Phys. Rev. B* **1**, 1184 (1970).

⁶ G. Paul and H. E. Stanley, "Partial Test of the University Hypothesis: The Case of Next-Nearest-Neighbor Interactions," *Phys. Rev. B* **5**, 3715 (1972).

2. FREE ENERGY

The Helmholtz free energy, F , of the Ising model can be written^{7,8} as

$$-\beta F = -L[\rho \ln \rho + (1-\rho) \ln (1-\rho)] + \sum_{\text{Sites}} \sum_{D'} D', \quad (1)$$

where β is the usual Boltzmann temperature factor, $1/(kT)$; ρ is the density (fraction of sites that are occupied), and D' is the set of topologically distinct connected diagrams composed of interaction bonds and density dependent vertices. Any number of bonds can connect sites i and j ; the weight to be assigned such a bond is (βJ_{ij}) if $i \neq j$ and 0 if $i = j$, where J_{ij} is the interaction energy between particles on these sites. The weight factor associated with a vertex is a polynomial in the density whose coefficients depend on the "kind of articulation vertex" that is under consideration. An articulation vertex is of the p th kind (or order) if its removal would cause the diagram to separate into p disjoint parts. The simplest example of an articulation vertex is the central vertex in a star diagram composed of dumbbells that are joined at (or share) a common vertex (see Fig. 1). Such a vertex is of the s th kind if there are s points to the star.

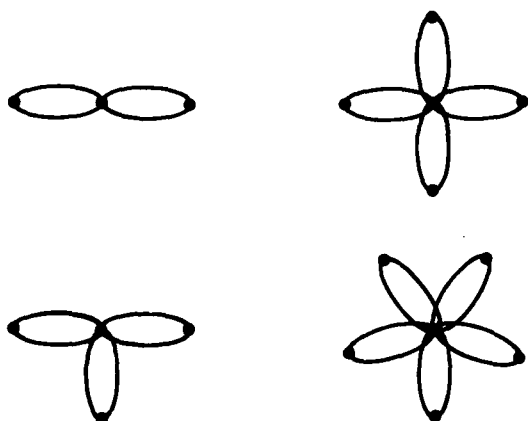


Figure 1—Simple examples of diagrams with articulated vertices: $\nu > 1$.

The usual virial expansion of the free energy involves the sum of more than singly connected single-bonded diagrams composed of vertices having weight ρ interconnected by bonds b_{ij} and $-\delta_{ij}$. Here, single-bonded means that no more than one bond can connect a pair of vertices; $b_{ij} = [\exp(\beta J_{ij}) - 1]$; and δ_{ij} is 1 if $i = j$, and is 0 if $i \neq j$. Equation 1 is obtained^{7,9} by: (1) Taylor series expanding the factor $[\exp(\beta J_{ij}) - 1]$, which leads to multiple (βJ_{ij}) -bonds and a symmetry factor to account for the interchangeability of the multiple bonds that connect a pair of vertices; (2) using the well-known result for the hard core gas to evaluate the sum of diagrams that do not contain (βJ_{ij}) -bonds; (3) demonstrating that there is an exact cancellation among the set of diagrams that contain b_{ij} -bonds and have one or more vertices that do not have at least one b_{ij} -bond emanating from them; and (4) introducing density weight factors to accomplish a vertex renormalization, i.e., to sum over $-\delta_{ij}$ -bond configurations. The density weight factor for an articulation vertex of the ν th kind is denoted by $M_{n_1, n_2, \dots, n_\nu}$, where n_i is the number of bonds that connect the vertex to the i th disjoint part into which the diagram would separate if the vertex were removed. Step 3 demonstrates that each vertex, ρ , has one or more b_{ij} bonds emanating from it, so that the weight factor is a polynomial in the density of order of the number of

bonds emanating from the circle, i.e., of order $\sum_{i=1}^{\nu} n_i$.

The density weight factor for articulation vertices of the first, second, and third kind have been obtained⁸ from recurrence relations among their coefficients. A detailed description of the derivation of the recurrence relations is given in Ref. 7. The generating functions that lead to these relationships are a direct consequence of a diagrammatic theorem⁷ that expresses the density weight factors for vertices of higher kind in terms of sums of products of density weight factors of lower kinds. This theorem, or zero sum rule, states that the contribution of the diagram representing $M_{n_1, n_2, \dots, n_\nu}$ plus the contributions of all its associated diagrams sum to zero. The associated

⁷ R. A. Farrell, T. Morita, and P. H. E. Meijer, "Cluster Expansion for the Ising Model," *J. Chem. Phys.* **45**, 349 (1966).

⁸ P. Esfandiari, P. H. E. Meijer, R. A. Farrell, and S. Favin, "New Generating Functions and Results for the Density Polynomials of the Lattice Gas," *Phys. Rev. B* **24**, 1298 (1981).

also, "Erratum: New Generating Functions and Results for the Density Polynomials of the Lattice Gas," *Phys. Rev. B* **25**, 6030 (1982).

⁹ T. Morita and K. Hiroike, "A New Approach to the Theory of Classical Fluids, III—General Treatment of Classical Systems," *Prog. Theor. Phys.* **25**, 537 (1961).

diagrams are constructed as follows. The ν disjoint parts into which the diagram would separate if this circle were removed are represented by ν labeled black triangles on a field (compare Fig. 2). Open p -gons ($p = 2$ is a circle, $p = 3$ a triangle, etc.) are inserted between the black triangles in all possible combinations. Inside each p -gon are one or more black dots that are connected to the black triangles by bonds of weight 1. The following three rules must be obeyed: (1) each black triangle is not articulated, and black triangle i has exactly n_i bonds emanating from it, (2) each black dot within a given p -gon is connected to p specific black triangles, and (3) the number of black dots within a p -gon is only restricted by the constraint that it obey these rules.

This classification is trivial for $\nu = 2$, and for $\nu = 3$ it generates the five types of diagrams shown in Fig. 2. The evaluation of these generic diagrams produces the generating functions given in Ref. 7. We

have used analogous classifications to construct the sets of associated diagrams for each of the density weight factors of the fourth and fifth kind needed to calculate the free energy through tenth order in inverse temperature. The use of specific n_i 's simplifies the procedure by eliminating certain generic diagrams that would occur for larger n_i 's. In order to illustrate this simplification, consider what would happen if we had listed the associated diagrams for the $\nu = 3$ case of $M_{2,2,2}$. Because only two bonds would emanate from each star, neither the second nor the third types of generic diagrams in Fig. 2 would appear in the list. Analogous exclusions occur for $\nu = 4$ and 5. In Ref. 7, the procedure was illustrated by listing the diagrams for the case of $M_{2,2,2,2,2}$. In this report, we list all of the required diagrams in Figs. 3 through 7. From these figures and the generating functions derived in Ref. 7, one obtains the density weight factors listed in Table 1.

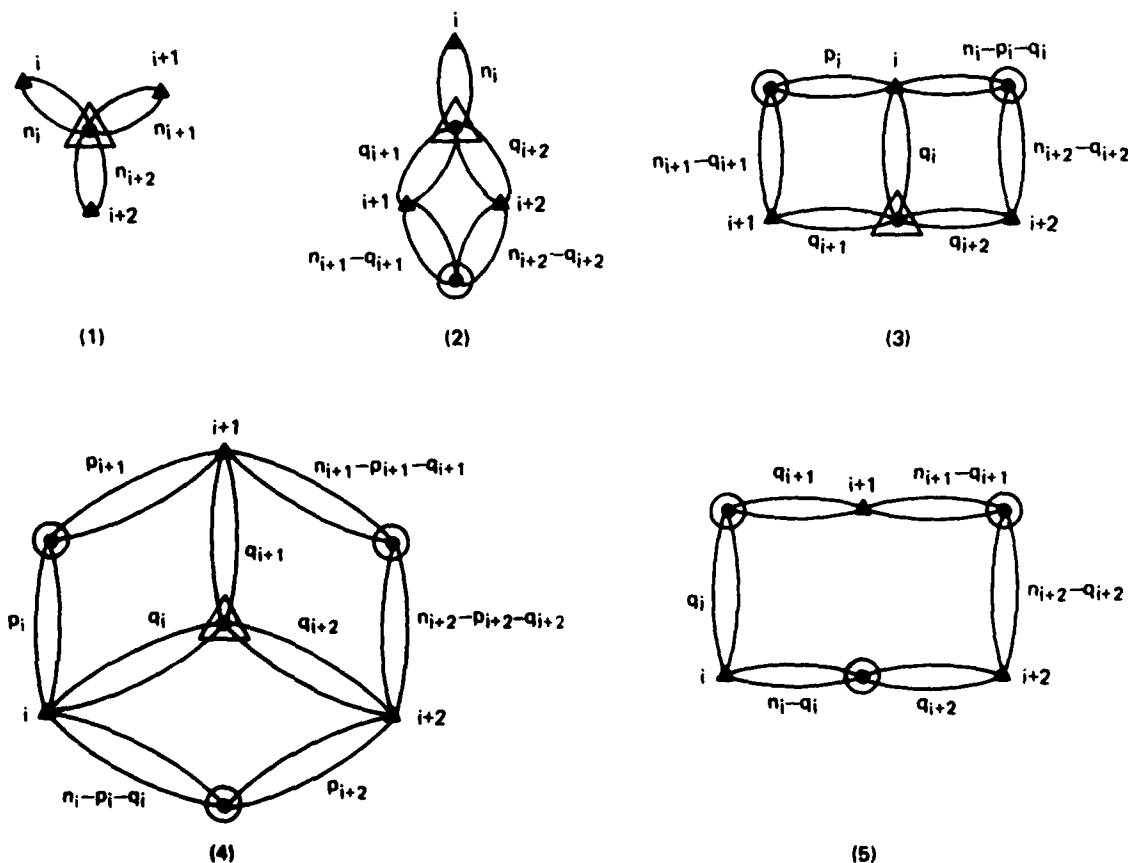


Figure 2—The five generic diagrams generated by the $\nu = 3$ sum rule.

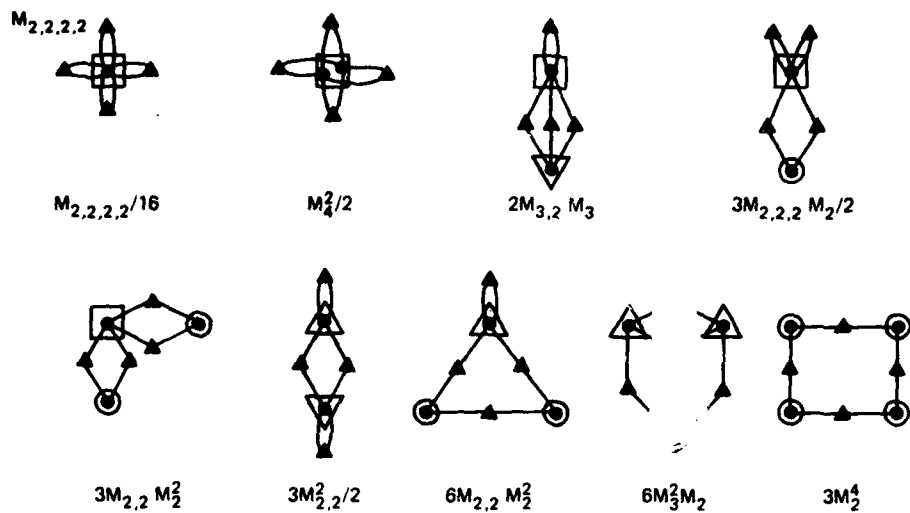


Figure 3—The diagrams that contribute to $M_{2,2,2,2}$.

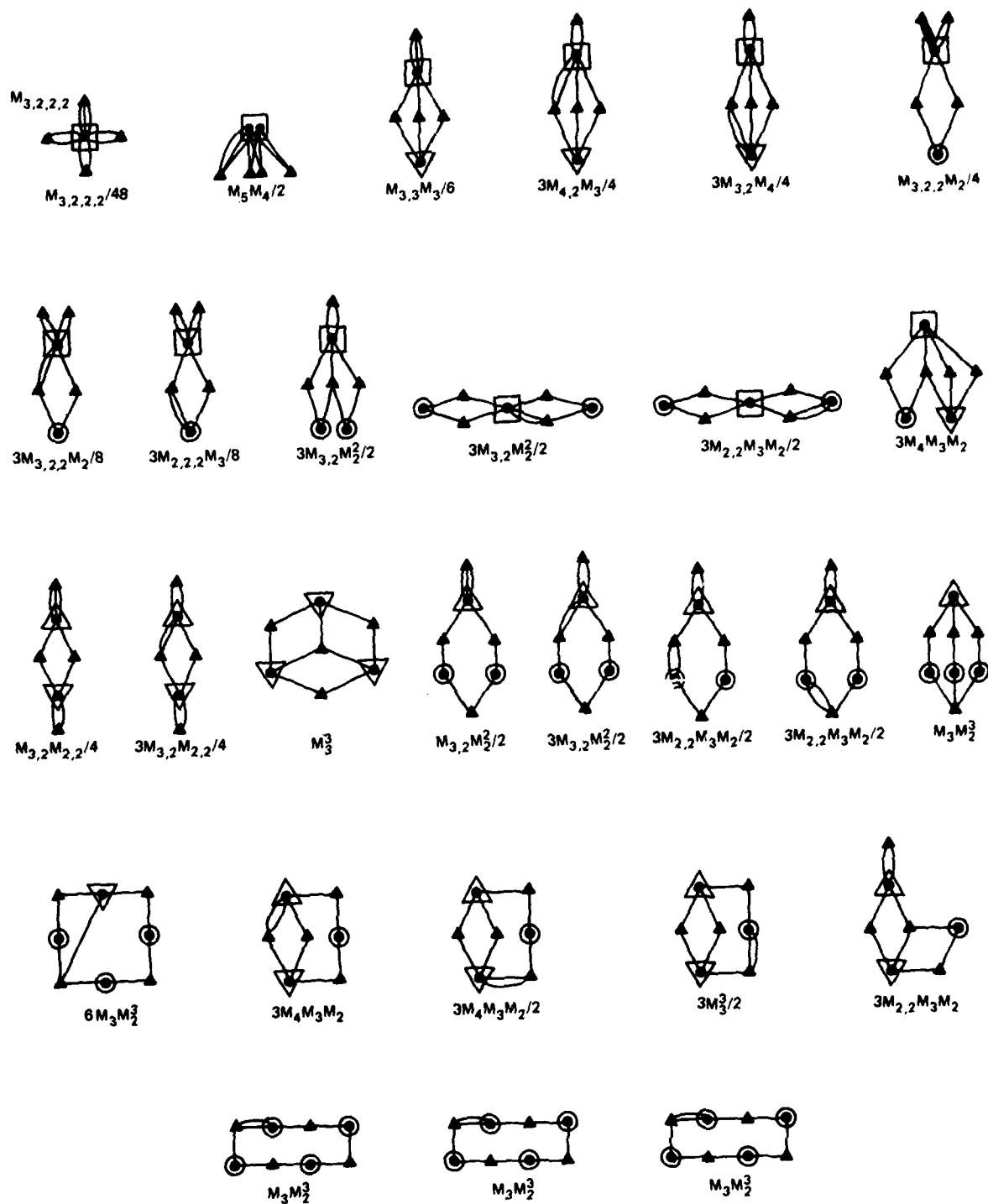
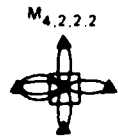


Figure 4—The diagrams that contribute to $M_{3,2,2,2}$.



$M_{4,2,2,2}/192$



$M_6 M_4/6$



$M_5^2/8$



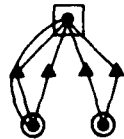
$M_{4,3} M_3/24$



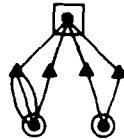
$M_{5,2} M_3/4$



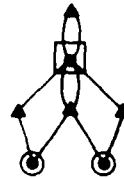
$3M_{4,2} M_4/8$



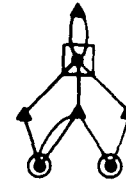
$3M_{3,2} M_3 M_2/4$



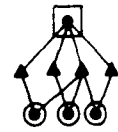
$M_{2,2} M_4 M_2/2$



$3M_{4,2} M_2^2/4$



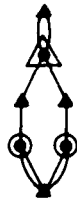
$3M_{3,2} M_3 M_2/2$



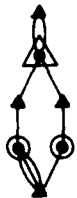
$M_4 M_2^3$



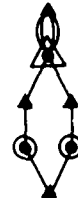
$3M_5 M_3 M_2$



$3M_{2,2} M_3^2/8$



$M_{2,2} M_4 M_2/2$



$M_{4,2} M_2^2/8$



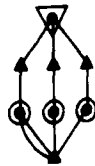
$M_{2,2} M_4 M_2/2$



$3M_2 M_{3,2} M_3/4$



$M_{4,2} M_2^2/2$



$3M_3^2 M_2^2/2$



$3M_5$



$M_3^2 M_4/2$



$3M_5$

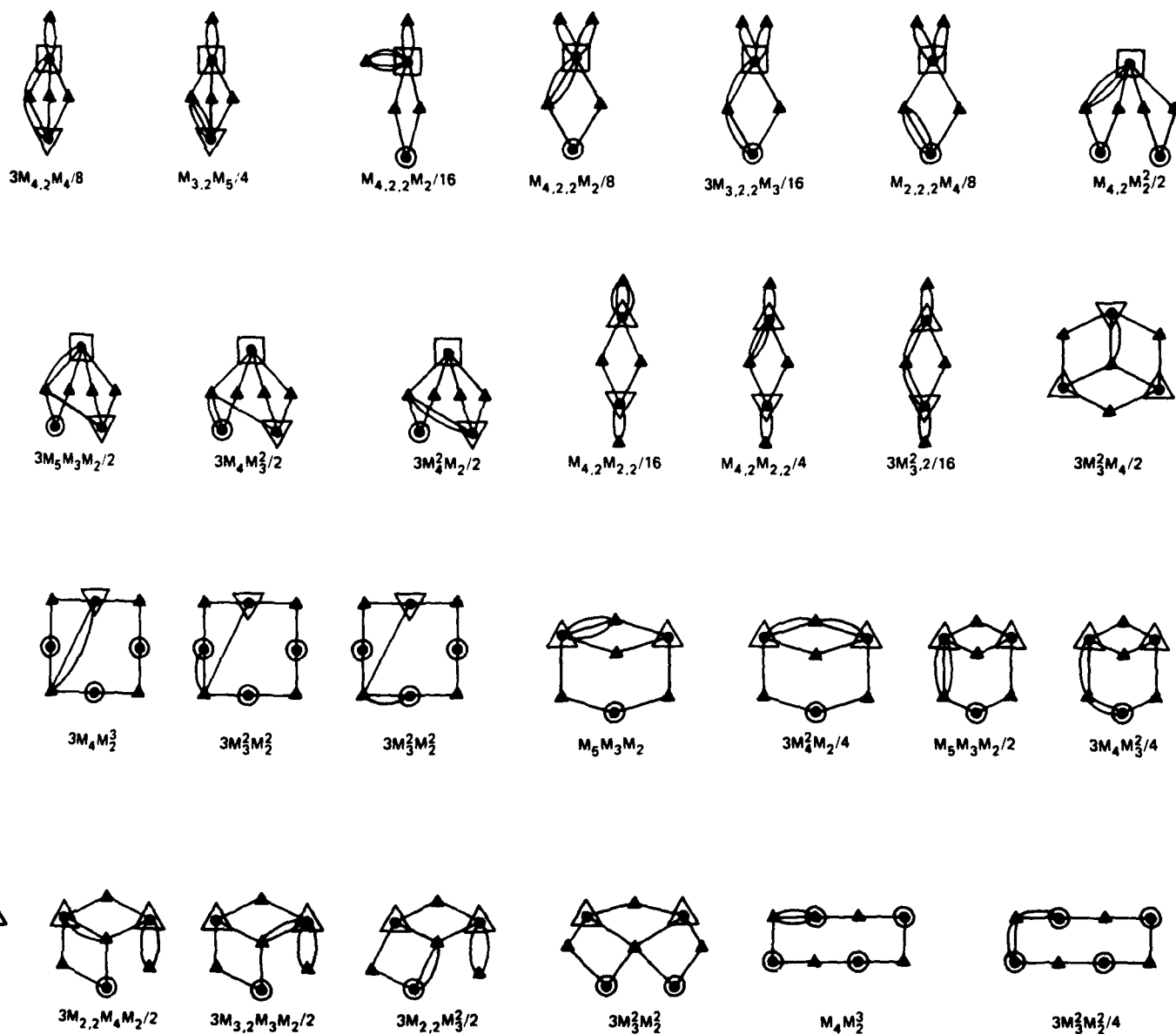
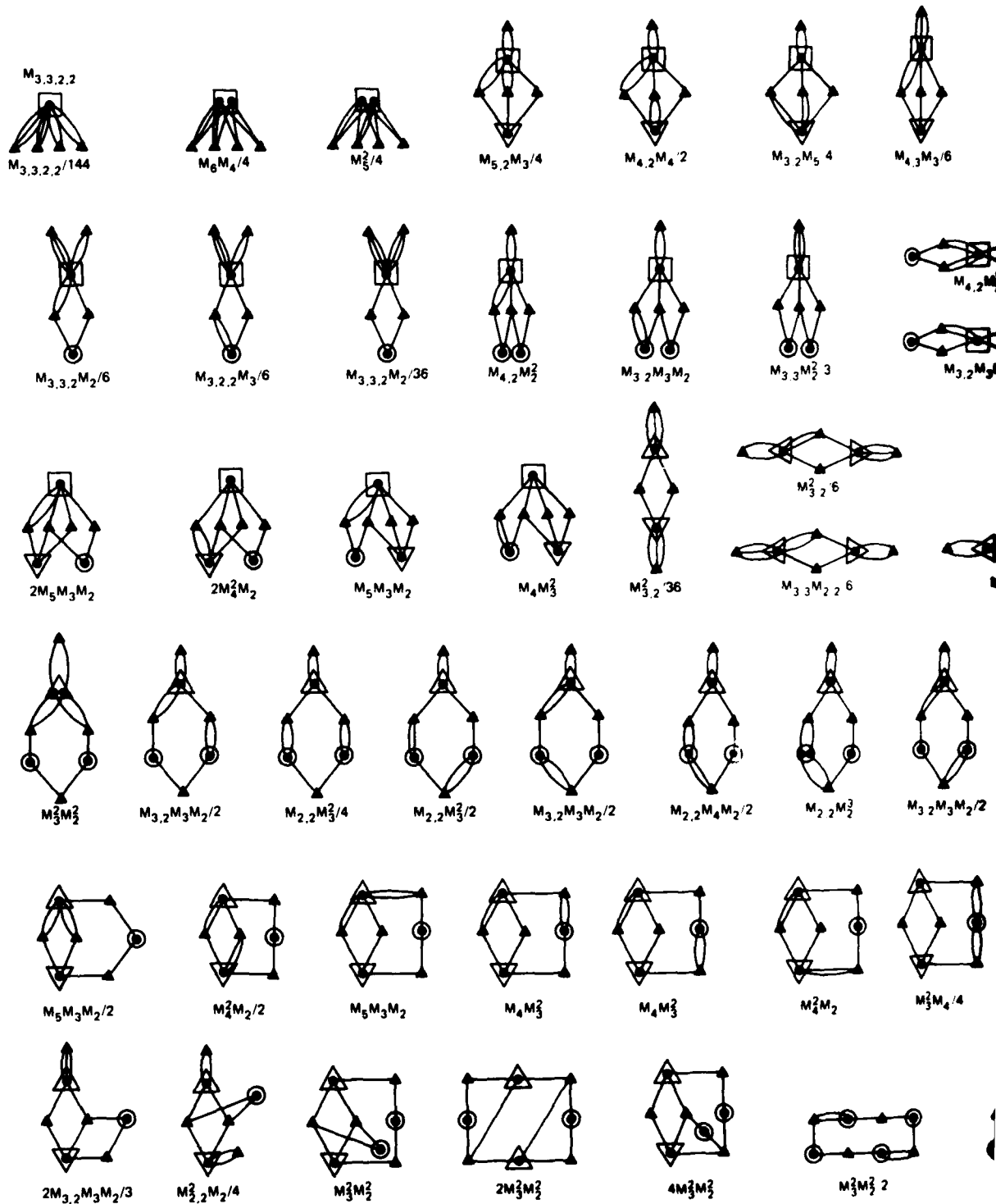


Figure 5—The diagrams that contribute to $M_{4,2,2,2}$.



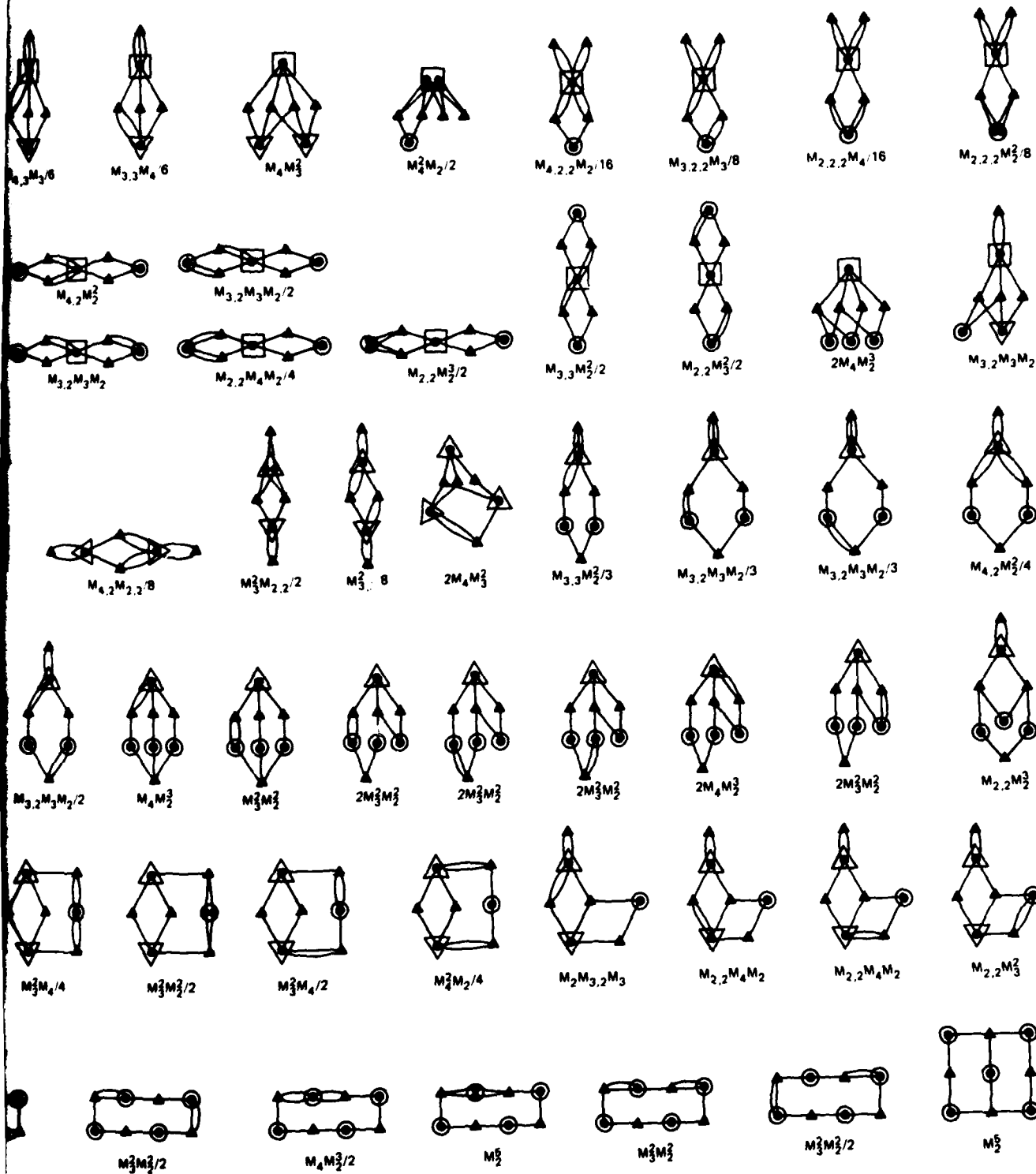


Figure 6—The diagrams that contribute to $M_{3,3,2,2}$.

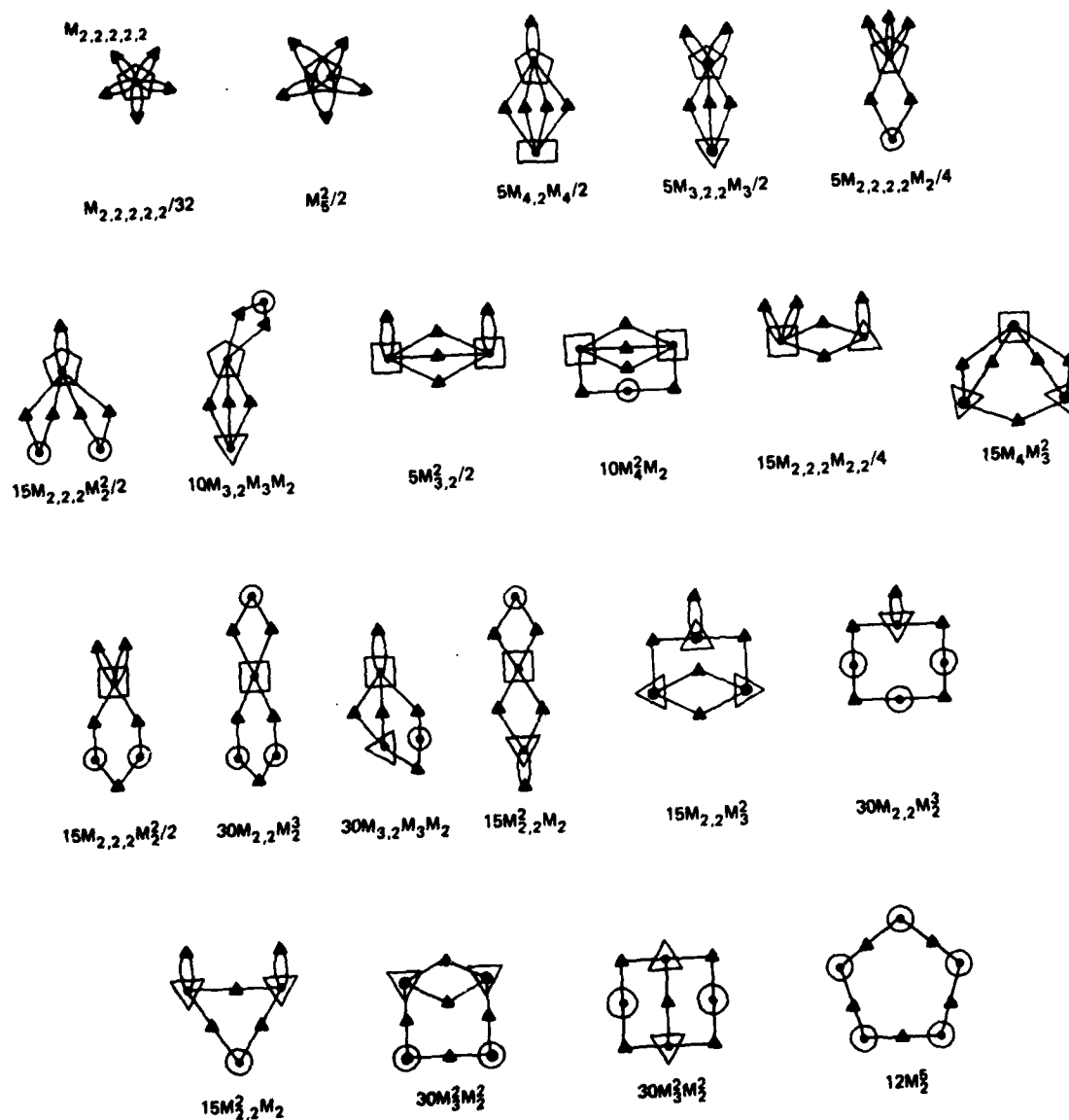


Figure 7—The diagrams that contribute to $M_{2,2,2,2,2}$.

Table 1—The coefficients $W_{n_1, n_2, \dots, n_r, m}$ in

1	0	0	0	0	1	0	0	0
2	0	0	0	0	1	-1	0	0
3	0	0	0	0	1	-3	2	0
4	0	0	0	0	1	-7	12	-6
5	0	0	0	0	1	-15	50	-60
6	0	0	0	0	1 -120	-31 0	180 0	-390 0
7	0	0	0	0	1 -2520	-63 720	602 0	-2100 0
8	0	0	0	0	1 -31920	-127 20160	1932 -5040	-10206 0
9	0	0	0	0	1 -317520	-255 332640	6050 -181440	-46620 40320
10	0	0	0	0	1 -2739240	-511 4233600	18660 -3780000	-204630 1814400
2	2	0	0	0	0	-2	4	-2
3	2	0	0	0	0	-6	24	-30
3	3	0	0	0	0 -84	-18 0	120 0	-270 0
4	2	0	0	0	0 -72	-14 0	100 0	-230 0
4	3	0	0	0	0 -2016	-42 576	456 0	-1650 0
4	4	0	0	0	0 -28224	-98 17856	1636 -4464	-6882 0
5	2	0	0	0	0 -1680	-30 480	360 0	-1350 0
5	3	0	0	0	0 -27300	-90 17280	1560 -4320	-8550 0
5	4	0	0	0	0 -294000	-210 308640	5400 -168480	-42570 37440
5	5	0	0	0	0 -2622900	-450 4060800	17400 -3628800	-193950 1742400
6	2	0	0	0	0 -22680	-62 14400	1204 -3600	-6902 0
6	3	0	0	0	0 -282240	-186 296640	5064 -162000	-40536 36000
6	4	0	0	0	0 -2599632	-434 4026240	17140 -3598560	-191816 1728000
7	2	0	0	0	0 -235200	-126 248640	3864 -136080	-32536 30240
7	3	0	0	0	0 -2494884	-378 3870720	15960 -3462480	-18207 166320
8	2	0	0	0	0 -2088072	-254 3265920	12100 -2933280	-14598 141120

As $W_{n_1, n_2, \dots, n_p, m}$ in the density weight factor polynomial $M_{n_1, n_2, \dots, n_p} = \sum_{m=1}^{n_1+n_2+\dots+n_p} W_{n_1, n_2, \dots, n_p, m} \rho^m$.

0	0	2	2	2	0	0	0	-4	40	-100	96
0	0						-32	0	0	0	0
0	0	3	2	2	0	0	0	-12	192	-780	1320
-6	0						-1008	288	0	0	0
-60	24	3	3	2	0	0	0	-36	864	-5220	13608
-390	360						-17640	11232	-2808	0	0
0	0	3	3	3	0	0	0	-108	3744	-31860	118584
-2100	3360						-225824	242784	-132840	29520	0
0	0	4	2	2	0	0	0	-28	712	-4444	11760
-10206	25200						-15344	9792	-2448	0	0
0	0	4	3	2	0	0	0	-84	3072	-27060	102552
-46620	166824						-200592	212832	-116640	25920	0
40320	0	4	3	3	0	0	0	-252	12960	-155340	802872
-204630	1020600						-2191896	3417120	-3063960	1473120	-294624
1814400	-362880	4	4	2	0	0	0	-196	10600	-131620	694176
							-1916768	3006720	-2704320	1901760	-260352
		5	2	2	0	0	0	-60	2400	-22140	85800
							-169680	180960	-99360	22080	0
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0	0						-8064	5184	-1296	0	0
-1650	2676	3	2	2	2	0	0	-24	1344	-13800	55920
0	0						-112896	121536	-66960	14880	0
-8882	22176	3	3	2	2	0	0	-72	5760	-81720	456624
0	0						-1297296	2064960	-1870560	902880	-180576
-1350	2220	4	2	2	2	0	0	-56	4720	-69320	395136
0	0						-1135008	1817280	-1650960	797760	-159552
-8550	21420	2	2	2	2	2	0	-16	2080	-35920	220416
0	0						-656768	1071360	-982080	476160	-95232
-42570	153780										
37440	0										
-193950	973980										
1742400	-348480										
-6902	17640										
0	0										
-40530	147252										
36000	0										
-191810	944656										
1728000	-345600										
-32550	121212										
30240	0										
-182070	922572										
1663200	-332640										
-145910	760536										
1411200	-282240										

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3. APPLICATION TO THE NEAREST NEIGHBOR MODEL

In order to determine the free energy we constructed two sets of lattice diagrams. The first set consists of all connected and nonarticulated diagrams that have 10 or fewer bonds. There are 185 single-bonded diagrams of this type; they are listed in Fig. 8, together with their symmetry numbers. The free multiplicities of these diagrams for nearest-neighbor models on the cubic lattices are presented in Tables 2 and 3. They are in accord with the recently published tables of Kincaid, Baker, and Fullerton.¹⁰ The exclusion of triangular, pentangular, etc. figures on the simple-cubic and body-centered-cubic lattices greatly reduces the number of diagrams needed for those cases.

The second set of lattice diagrams consists of all the articulated diagrams with 10 or fewer bonds. These are generated by joining together two or more nonarticulated diagrams at one or more common vertices. In constructing these diagrams, one uses all the previously listed nonarticulated diagrams except that the single-bonded two-vertex diagram (i.e., the single-bonded dumbbell) cannot occur as an element emanating from a vertex; such a diagram element has to be at least double-bonded. This exclusion is a consequence of the fact that the articulation vertices are formed by collapsing a number of vertices (that were connected by δ_{ij} -bonds). Subject to this restriction, we find that there are 245 topologically distinct articulated diagrams with the minimum number of bonds between their vertices; they are listed in Fig. 9, together with their symmetry numbers. The free multiplicity of an articulated diagram is simply the product of the free multiplicities of the nonarticulated diagram elements used to generate it; it has not been listed.

After these lists were composed and checked, we generated the additional terms by multiple-bonding all of the previously listed diagrams. Multiple-bonding does not change the number of ways the diagram fits into the lattice (i.e., its free multiplicity) but it does change the density weight factors, the order of the temperature contribution, and the symmetry number appropriate to the diagram. Multiple-bonding changes the symmetry of a diagram for two reasons. First, multiple-bonds that connect a given pair of vertices are equivalent; this is accounted for

by introducing a product of factorials in recognition of their interchangeability. The second reason is that the overall symmetry of the single-bonded diagram can be changed. For example, the symmetry number of a p -gon is $2p$ because there are p rotations and one flip of the diagram, each of which leads to a diagram that is topologically equivalent. If one of the pairs of connected points in a p -gon is joined by multiple bonds and the other $(p-1)$ connections are single-bonded, then the symmetry number is reduced to 2 because the rotations lead to topologically distinct diagrams; only the flip around the center of the multiple bonded pair leads to a topologically equivalent diagram. Usually one would account for this change of symmetry by listing only topologically distinct unlabeled diagrams and using their modified symmetry numbers. Alternatively, one can sum over all possible multiple bondings of the single-bonded diagram independently and use the overall symmetry number of the single-bonded diagram (modified by the product of factorials mentioned above). We have used this alternative because it is ideally suited for a computing machine. This procedure is based on the fact that independent multiple-bonding can lead to topologically equivalent diagrams, and the number of such diagrams of a given type is simply the ratio of the symmetry number of the single-bonded diagram to that of the multiple bonded diagram. A few simple examples are presented in Fig. 10.

We created the computer compilation program reproduced and annotated in the appendix in order to accumulate the contributions of the aforementioned 430 lattice diagrams and the needed multiple-bonded diagrams that they generate. The following information is used to characterize each diagram: an arbitrary label, 1 to 430; the symmetry number of the single-bonded diagram; the unrestricted lattice constant (i.e., free multiplicity) for the lattice under consideration; the total number of vertices, NC ; the total number of bonds (actually, the number of connected pairs of vertices), NB , in the single-bonded diagram; and two sequences of numbers to specify the diagram's topology (i.e., the manner in which the vertices are interconnected). The first sequence gives the lower limits on the number of bonds between each of the NB pairs of vertices that are connected. These numbers are in general equal to unity, except in the case of a two-vertex element (dumbbell) in an articulated diagram where the number is 2 (for the reasons discussed above). The second sequence of numbers consists of two subsets. The first subset

¹⁰ J. M. Kincaid, G. A. Baker, Jr., and L. W. Fullerton, "High-Temperature Series Expansions of the Continuous-Spin Ising Model," Los Alamos Scientific Report La-Ur-79-1575 (unpublished).

specifies the articulation order of each of the NC vertices; i.e., it is a sequence of NC numbers that are unity if the vertex is nonarticulated, 2 if the articulation is of the second kind, etc. The second subset gives the emanation numbers of each vertex. If the vertex is nonarticulated, there is only one set of emanation numbers that specify the other vertices to which it is connected. If it is an articulation vertex of the p th kind, there are p sets of emanation numbers needed because the diagram separates into p elements if the vertex is removed. In this case, each set of emanation numbers specifies those vertices within a particular one of the p elements that are connected to the vertex of interest. This scheme, cumbersome as it may seem, is a very efficient way to transfer the information into the code. The data were proofread several times and were checked by using them to regenerate the diagram.

The program takes these data for a single-bonded diagram, generates the labels of the appropriate density weight factors, multiplies these NC polynomials together, and multiplies the result by the ratio of the free multiplicity divided by the symmetry number. The final result is then accumulated in the appropriate

ate $C_{n,m}$, where

$$-\beta F = -L[\rho \ell n \rho + (1-\rho) \ell n(1-\rho)] \\ + \sum_{n=1}^{10} \sum_{m=1}^{2n} C_{n,m} \rho^m (J/kT)^n + O[(J/kT)^{11}]. \quad (2)$$

Next, the program automatically multiple-bonds the diagram and repeats the procedure. The free energy series for the three cubic lattices are given in Tables 4 through 6. These coefficients were compared with the results available in the literature. In particular, for the simple-cubic and body-centered-cubic lattices, the low temperature series of Sykes, Essam, and Gaunt¹¹ were used to determine the high temperature series by means of an inversion of the activity series into a density series. For the face-centered-cubic lattice, McKenzie's recent results¹² for the low temperature series were inverted. Exact agreement is found in all cases. Thus, we are confident that the symmetry numbers and density weight factors are correct. The evaluation of Eq. 1 for more general models (e.g., longer ranged interactions, multiple sublattice long range order parameters, etc.) are under way.

¹¹ M. F. Sykes, J. W. Essam, and D. S. Gaunt, "Derivation of Low-Temperature Expansions for the Ising Model of a Ferromagnet and an Antiferromagnet," *J. Math. Phys.* 6, 283 (1965).

¹² S. McKenzie, "Extended High Temperature Low Field Expansions for the Ising Model," *Can. J. Phys.* 57, 1239 (1979).

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Lab	S	Lab	S	Lab	S	Lab	S				
1		2	21		2	41		4	61		1
2		6	22		48	42		1	62		6
3		8	23		4	43		2	63		4
4		4	24		8	44		2	64		6
5		10	25		4	45		2	65		2
6		24	26		4	46		2	66		4
7		12	27		2	47		4	67		2
8		2	28		2	48		4	68		4
9		12	29		2	49		2	69		12
10		2	30		4	50		2	70		2
11		12	31		4	51		4	71		8
12		4	32		16	52		2	72		12
13		2	33		18	53		2	73		8
14		4	34		20	54		2	74		12
15		4	35		2	55		1	75		48
16		14	36		2	56		4	76		2
17		4	37		4	57		2	77		2
18		8	38		1	58		6	78		4
19		1	39		1	59		72	79		2
20		2	40		2	60		12	80		4

S	Lab		S	Lab		S	Lab		S	Lab		S	Lab		S	Lab		S
1	81		2	101		2	121		1	141		2	161		2	181		2
6	82		4	102		8	122		2	142		1	162		4	182		2
4	83		2	103		12	123		2	143		2	163		4	183		2
6	84		2	104		2	124		1	144		1	164		2	184		2
2	85		8	105		8	125		2	145		1	165		4	185		2
4	86		4	106		16	126		4	146		4	166		2			
2	87		2	107		8	127		1	147		1	167		8			
4	88		1	108		2	128		2	148		1	168		2			
12	89		2	109		12	129		4	149		1	169		4			
2	90		4	110		6	130		1	150		1	170		4			
8	91		2	111		12	131		2	151		2	171		2			
12	92		2	112		4	132		4	152		2	172		2			
8	93		2	113		8	133		8	153		1	173		2			
12	94		16	114		120	134		8	154		2	174		4			
48	95		10	115		240	135		4	155		2	175		2			
2	96		2	116		2	136		2	156		1	176		1			
2	97		2	117		1	137		4	157		2	177		2			
4	98		12	118		1	138		1	158		1	178		1			
2	99		2	119		1	139		1	159		4	179		1			
4	100		4	120		4	140		4	160		2	180		2			

Figure 6—A complete list of more than simply connected diagrams with 10 or fewer bonds.

Table 2—The free multiplicities for the simple-cubic and body-centered-cubic lattices.

<u>L</u>	<u>FM</u> <u>sc</u>	<u>FM</u> <u>bcc</u>	<u>L</u>	<u>FM</u> <u>sc</u>	<u>FM</u> <u>bcc</u>
1	6	8	105	18612	140608
3	90	216	106	18612	140608
7	318	1000	109	20250	157464
9	1860	8000	115	8166	39304
14	1350	5832	128	20250	157464
22	1494	5832	129	18324	140608
24	960	4096	131	16134	125000
30	5712	32768	132	20250	157464
32	44730	343000	135	129330	1331000
34	1172556	16003008	137	108600	1124864
36	27900	216000	186	36	64
59	642	2744	187	216	512
64	3804	21952	188	216	512
67	4770	27000	189	1296	4096
69	22632	175616	190	1296	4096
85	4044	21952	191	1296	4096
86	3102	17576	192	7776	32768
103	24216	175616	193	7776	32768

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Table 3—The free multiplicities for the face-centered-cubic lattice.

<u>L</u>	<u>FM</u>	<u>L</u>	<u>FM</u>	<u>L</u>	<u>FM</u>	<u>L</u>	<u>FM</u>	<u>L</u>	<u>FM</u>
1	12	38	69120	75	3072	112	49344	149	47520
2	48	39	97200	76	34560	113	768	150	48384
3	540	40	69120	77	34560	114	0	151	36336
4	192	41	66816	78	34560	115	268044	152	58752
5	4320	42	74304	79	30728	116	675840	153	35328
6	48	43	69120	80	49344	117	777600	154	58752
7	3084	44	97200	81	51360	118	777600	155	38064
8	2160	45	97200	82	28176	119	675840	156	34560
9	42240	46	83520	83	49344	120	602880	157	25920
10	768	47	102816	84	49344	121	688704	158	35328
11	768	48	1770240	85	107088	122	563760	159	36336
12	1056	49	1452096	86	75372	123	675840	160	34560
13	17280	50	2928	87	35328	124	777600	161	34560
14	24300	51	4224	88	34560	125	777600	162	28368
15	19728	52	3072	89	49344	126	675840	163	47520
16	403200	53	3072	90	42624	127	777600	164	37248
17	192	54	5136	91	49344	128	1093500	165	25920
18	384	55	4224	92	768	129	1015632	166	47520
19	8640	56	2160	93	1536	130	669888	167	47808
20	8640	57	4224	94	2976	131	838380	168	785088
21	12336	58	3072	95	960	132	1093500	169	13059648
22	25740	59	8412	96	1056	133	679536	170	675840
23	8640	60	3792	97	1776	134	567168	171	1110240
24	14688	61	78912	98	2592	135	17473500	172	783552
25	8640	62	59328	99	1536	136	13639680	173	783552
26	6480	63	97200	100	2976	137	13971072	174	887760
27	8832	64	104112	101	768	138	34560	175	887760
28	168960	65	78912	102	768	139	34560	176	783552
29	194400	66	78912	103	1361136	140	17280	177	777600
30	195888	67	138780	104	766512	141	36000	178	887760
31	155952	68	69120	105	978240	142	28128	179	623808
32	4038300	69	1468272	106	978240	143	25920	180	671904
33	40958400	70	3072	107	808704	144	25920	181	562176
34	423550512	71	8640	108	623808	145	35328	182	623808
35	1612800	72	130320	109	1093500	146	25920	183	16153200
36	1900800	73	90624	110	102960	147	34560	184	18144000
37	1555200	74	48	111	34560	148	34560	185	15206400

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186	2	214	2	242	8	272	2
187	6	215	2	243	16	273	4
188	2	216	2	244	2	274	2
189	24	217	8	245	4	275	2
190	2	218	8	246	2	276	4
191	2	219	2	247	2	277	4
192	120	220	4	248	2	278	4
193	8	221	8	249	4	279	2
194	6	222	8	250	1	280	2
195	2	223	48	251	2	281	4
196	2	224	2	252	2	282	4
197	2	225	4	253	4	283	2
198	2	226	2	254	2	284	2
199	4	227	4	255	4	285	2
200	2	228	4	256	4	286	2
201	2	229	12	257	2	287	4
202	12	230	4	258	4	288	2
203	2	231	2	259	4	289	4
204	1	232	4	260	8	290	8
205	6	233	8	261	4	291	4
206	2	234	16	262	2	292	4
207	4	235	4	263	4	293	6
208	8	236	8	264	2	294	12
209	2	237	8	265	4	295	6
210	8	238	2	266	4	296	12
211	4	239	2	267	2	297	4
212	16	240	4	268	4		
213	4	241	2	269	4		

S	Lab		S	Lab		S	Lab		S	Lab		S	Lab		S
8	298		12	326		1	354		8	382		1	411		2
4	299		4	327		1	355		4	383		1	412		2
4	300		6	328		1	356		4	384		1	413		1
1	301		8	329		2	357		2	385		1	414		1
2	302		12	330		4	358		1	386		1	415		1
4	303		4	331		2	359		4	387		1	416		2
4	304		6	332		2	360		2	388		2	417		1
2	305		8	333		2	361		2	389		1	418		1
2	306		12	334		4	362		1	390		1	419		1
4	307		2	335		2	363		1	391		2	420		2
2	308		4	336		4	364		2	392		2	421		4
4	309		12	337		4	365		4	393		2	422		2
4	310		8	338		2	366		2	394		1	423		2
2	311		12	339		2	367		2	395		2	424		2
2	312		2	340		4	368		4	396		2	425		1
2	313		1	341		2	369		2	397		24	426		2
2	314		1	342		1	370		2	398		12	427		4
4	315		4	343		1	371		2	399		2	428		2
2	316		2	344		2	372		4	400		2	429		4
4	317		2	345		4	373		4	401		2	430		2
8	318		2	346		2	374		4	402		4			
4	319		1	347		4	375		2	403		2			
4	320		1	348		6	376		4	404		2			
6	321		4	349		8	377		4	405		1			
12	322		2	350		12	378		2	406		2			
6	323		2	351		4	379		2	407		2			
12	324		1	352		2	380		8	408		2			
4	325		2	353		2	381		2	409		1			
										410		1			

Figure 9—Articulated single-bonded diagrams with 10 or fewer bonds subject to the dumbbell rule.

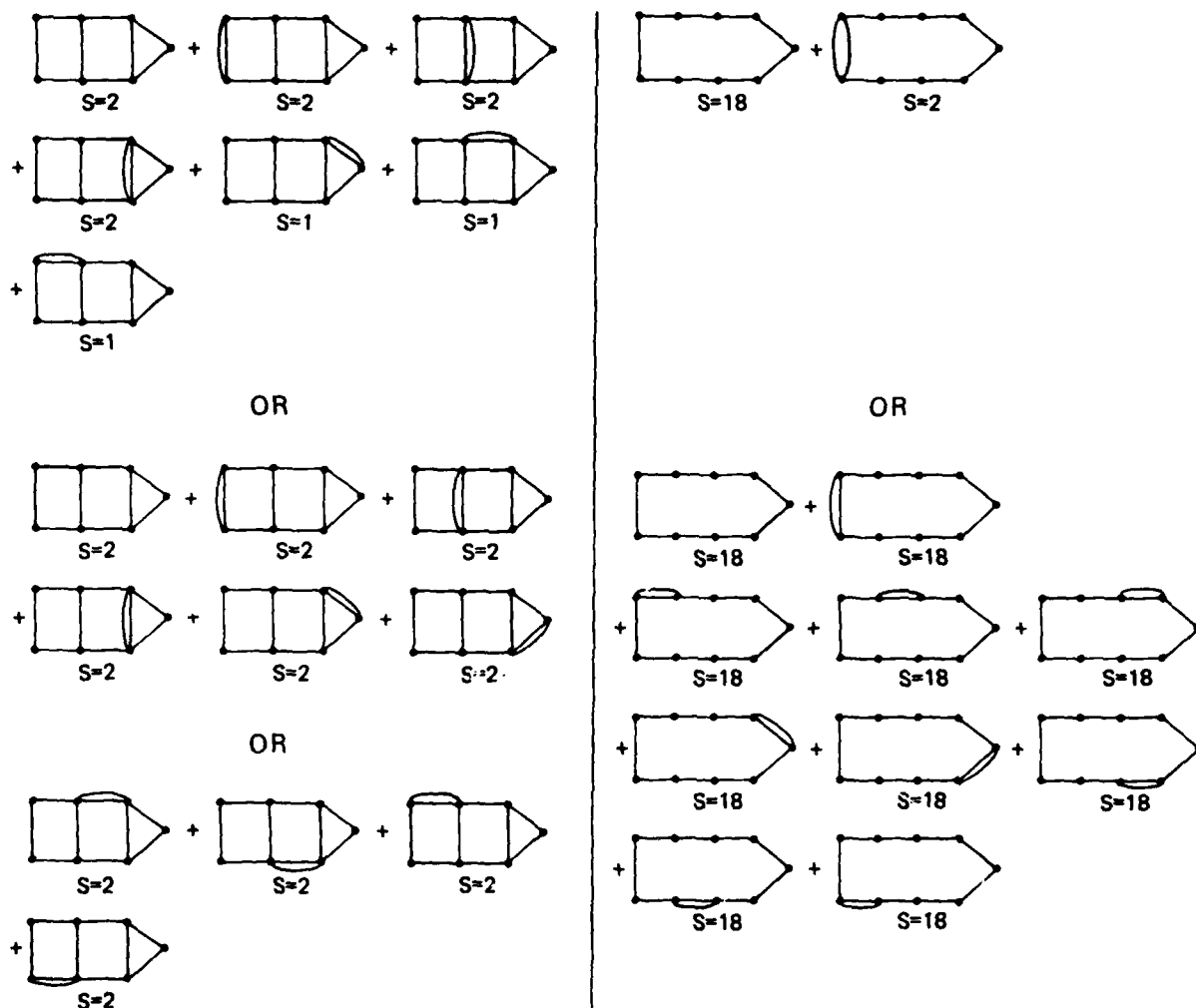


Figure 10—Examples of the two alternate ways of multiple-bonding a diagram. (As discussed in the text, the first method uses only topologically distinct diagrams and their associated symmetry numbers. The alternative procedure, which was used, does the multiple-bonding independently and uses only the symmetry number of the single-bonded diagram. The advantage of this alternative is that it is trivial to implement on the computer.)

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Table 4—The coefficients of $\rho^k (\beta J)^n$ in the Taylor-series expansion of the Helmholtz free energy of the nearest-neighbor lattice gas on the face-centered-cubic lattice. The entry $C(n, k) = ij:lm$ is to be read as $ij + [lm/(n!2)]$, e.g., $C(9, 8) = 21591:498960 = 215291 + 498960/(9!2) = 215291.6875$.

$k+n \rightarrow$	1	2	3	4	5	6	7	8	9	10
2	6:0	3:0	1:0	0:12	0:12	0:12	0:12	0:12	0:12	0:12
3	0:0	-6:0	2:0	8:24	8:120	5:696	2:7224	1:9048	0:284280	0:883416
4	0:0	3:0	-11:0	-34:12	-10:180	49:372	96:588	104:66036	84:613740	56:615252
5	0:0	0:0	12:0	57:0	-75:0	-374:720	-394:7056	158:17136	1042:344880	1765:2409840
6	0:0	0:0	-4:0	-54:0	285:96	1021:0	-149:4368	-4336:14112	-7039:495984	-1184:5724000
7	0:0	0:0	0:0	33:0	-468:0	-1495:0	4542:0	16482:30240	-6581:181440	-114154:5320800
8	0:0	0:0	0:0	-7:24	423:0	1225:1080	-14813:7920	-21321:7560	215291:498960	916676:3870360
9	0:0	0:0	0:0	0:0	-204:0	-480:0	26854:0	-33913:40320	-119307:544320	-4000948:3628800
10	0:0	0:0	0:0	0:0	40:192	8:0	-31784:0	193247:0	3419789:84672	11978410:4596480
11	0:0	0:0	0:0	0:0	0:0	48:0	25452:0	-39342:0	-7211599:0	-26568250:1451520
12	0:0	0:0	0:0	0:0	0:0	-8:0	-13446:0	476890:0	11052791:362880	45108674:5564160
13	0:0	0:0	0:0	0:0	0:0	0:0	4248:0	-371007:0	-12494314:0	-59478333:0
14	0:0	0:0	0:0	0:0	0:0	0:0	-606:8640	182406:0	10350458:0	61194742:0
15	0:0	0:0	0:0	0:0	0:0	0:0	0:0	-51762:0	-6122232:0	-48994063:4354560
16	0:0	0:0	0:0	0:0	0:0	0:0	0:0	6470:20160	2450285:0	30169646:1088640
17	0:0	0:0	0:0	0:0	0:0	0:0	0:0	0:0	-594708:0	-13920714:0
18	0:0	0:0	0:0	0:0	0:0	0:0	0:0	0:0	66078:483840	4565694:0
19	0:0	0:0	0:0	0:0	0:0	0:0	0:0	0:0	0:0	-953352:0
20	0:0	0:0	0:0	0:0	0:0	0:0	0:0	0:0	0:0	95335:1451520

Table 5—The coefficients of $\rho^k (\beta J)^n$ in the Taylor-series expansion of the Helmholtz free energy of the nearest-neighbor lattice gas on the body-centered cubic lattice.

$k+n \rightarrow$	1	2	3	4	5	6	7	8	9	10
2	4:0	0:8	0:8	0:8	0:8	0:8	0:8	0:8	0:8	0:8
3	0:0	-4:0	-4:0	-2:16	-1:0	-0:496	-0:1008	-0:2032	-0:4080	-0:6176
4	0:0	2:0	8:8	23:8	32:200	31:248	22:4424	13:9752	6:365000	2:5879768
5	0:0	0:0	-8:0	-74:0	-230:0	-368:480	-390:2016	-306:74592	-189:673440	-94:5503200
6	0:0	0:0	2:8	104:0	716:224	2070:960	3631:6272	4599:51072	4630:64544	3934:3004800
7	0:0	0:0	0:0	-68:0	-1192:0	-6523:480	-19593:3360	-39780:68544	-60576:201600	-73531:2212800
8	0:0	0:0	0:0	17:0	1102:0	12336:1200	64691:4800	209144:17136	471586:110880	801956:4242480
9	0:0	0:0	0:0	0:0	-536:0	-14353:480	-136674:6720	-709859:26880	-2376364:524160	-5687290:2217600
10	0:0	0:0	0:0	0:0	107:48	10086:960	189061:3360	1620446:53760	8157048:459648	27714932:927360
11	0:0	0:0	0:0	0:0	0:0	-3936:0	-170832:0	-2543142:0	-19688292:0	-96122683:1451520
12	0:0	0:0	0:0	0:0	0:0	656:0	97320:0	2755277:0	34019431:241920	242926042:967680
13	0:0	0:0	0:0	0:0	0:0	0:0	-31776:0	-2028222:0	-42324389:241920	-453899786:0
14	0:0	0:0	0:0	0:0	0:0	0:0	4539:4320	369876:0	37643736:0	630878500:0
15	0:0	0:0	0:0	0:0	0:0	0:0	0:0	-272052:0	-23371461:241920	-650529826:2903040
16	0:0	0:0	0:0	0:0	0:0	0:0	0:0	34006:40320	9629247:241920	491061591:725760
17	0:0	0:0	0:0	0:0	0:0	0:0	0:0	0:0	-2637464:0	-263758596:0
18	0:0	0:0	0:0	0:0	0:0	0:0	0:0	0:0	263051:403200	95496836:0
19	0:0	0:0	0:0	0:0	0:0	0:0	0:0	0:0	0:0	-20902208:0
20	0:0	0:0	0:0	0:0	0:0	0:0	0:0	0:0	0:0	2090220:5806080

Table 6—The coefficients of $\rho^k (\beta J)^n$ in the Taylor-series expansion of the Helmholtz free energy of the nearest-neighbor lattice gas on the simple cubic lattice.

$k+n \rightarrow$	1	2	3	4	5	6	7	8	9	10
2	3:0	0:6	0:6	0:6	0:6	0:6	0:6	0:6	0:6	0:6
3	0:0	-3:0	-3:0	-1:36	-0:180	-0:372	-0:756	-0:1524	-0:3060	-0:6132
4	0:0	1:2	6:6	11:18	12:150	10:546	6:8358	3:61746	1:576150	0:5473986
5	0:0	0:0	-6:0	-31:24	-76:120	-113:360	-119:6552	-98:51912	-67:21240	-38:6660360
6	0:0	0:0	2:0	42:0	225:168	603:0	1029:7224	1288:2016	1277:653208	1057:3679200
7	0:0	0:0	0:0	-27:0	-366:0	-1828:720	-5123:0	-9712:67536	-13853:393120	-15864:5190480
8	0:0	0:0	0:0	6:36	334:120	3374:900	15927:6120	46134:6804	94372:325080	148380:1978020
9	0:0	0:0	0:0	0:0	-162:0	-3870:0	-32313:0	-145814:20160	-431292:90720	-933449:907200
10	0:0	0:0	0:0	0:0	32:96	2699:0	43584:0	316910:60480	137987:102816	4140755:6683040
11	0:0	0:0	0:0	0:0	0:0	-1050:0	-38730:0	-481078:40320	-3156709:362880	-13354439:3084480
12	0:0	0:0	0:0	0:0	0:0	175:0	21873:0	509881:60480	5253431:544320	31931785:756000
13	0:0	0:0	0:0	0:0	0:0	0:0	-7116:0	-370198:40320	-6365135:0	-57232551:3628800
14	0:0	0:0	0:0	0:0	0:0	0:0	1016:5760	175653:0	5559771:0	77139645:0
15	0:0	0:0	0:0	0:0	0:0	0:0	0:0	-49107:0	-3411756:0	-77794745:5806080
16	0:0	0:0	0:0	0:0	0:0	0:0	0:0	6138:30240	1396200:362880	57820459:2358720
17	0:0	0:0	0:0	0:0	0:0	0:0	0:0	0:0	-342258:0	-30740634:0
18	0:0	0:0	0:0	0:0	0:0	0:0	0:0	0:0	38028:483840	11063145:0
19	0:0	0:0	0:0	0:0	0:0	0:0	0:0	0:0	0:0	-2415006:0
20	0:0	0:0	0:0	0:0	0:0	0:0	0:0	0:0	0:0	241500:4354560

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APPENDIX

THE COMPILATION PROGRAM

The notations used in this computer program are:

I	Diagram label.			quent labels are $[jao(j) - 1]$ out of sync. (This concept is illustrated below.)
S	Symmetry number.	NP	-(5,NNN)	Specifies the bonds that emanate from the vertex labeled by NNN . (Again, see below.)
W	Free multiplicity.			
NB	Number of connected vertex pairs.	IIT		Specifies the total number of bonds that can be added to a single-bonded diagram.
L - L(10); L(1), L(2), ..., L(NB)	The lower limit on the number of bonds between, respectively, the first, second, ..., and NB th vertex pair.	IjT		Specifies the upper limit on the number of bonds between the j th vertex pair.
INSLUM	The number of bonds in the single-bonded diagram.	INL	-	$L(N)$.
NC	The number of vertices (circles).			Figures A-1 and A-2 illustrate these conventions for two representative articulated diagrams.
JAO - JAO(NC); JAO(1), JAO(2), ..., JAO(NC)	The articulation orders of, respectively, the first, second, ..., and NC th vertex.			Lines 2 through 59 of the main program read in the data, identify the topology of the single-bonded diagram and prepare the do-loops to be used in multiple bonding. The integers $j_1, j_2, \dots, j_{NB}$ generated in lines 61 through 125 specify, respectively, the number of bonds between the first, the second, ..., and the NB th vertex pairs. Lines 126 through 168 obtain the indices, $N(III)$, for each of the circles, III ; identify the corresponding density weight factors; and multiplies them together. The multiplication of these polynomials is accomplished in a subroutine, POLYMT, which is also listed. Steps 169 through 214 accumulate the contributions to the coefficients $C_{n,m}$ of Eq. 2.
JAOSUM	The number of indices that must be specified in the product of polynomials (M 's).			The following pages list the compilation program.
NNN	Specifies the vertex label unless one (or more) of the vertices (say the j th) is articulated, in which case $jao(j)$ of the NNN 's are used for it and all subse-			

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C	EVALUATES ARTICULATION ISING DIAGRAMS.	S FAVIN	AUG 1982	MAIN	10
	IMPLICIT REAL*16(A-H,O-Z)			MAIN	20
	DIMENSION P(11,3,3,4,6,11), L(10), I(10), S1(21)			MAIN	30
	DIMENSION NP(5,10), JAO(10), N(5)			MAIN	40
	DIMENSION SS1(21,11)			MAIN	50
	DIMENSION ZZ(26136)			MAIN	60
	COMMON DEBUG			MAIN	70
	LOGICAL DEBUG			MAIN	80
	EQUIVALENCE (P(1,1,1,1,1,1), ZZ(1))			MAIN	90
	EQUIVALENCE (N(1),N1), (N(2),N2), (N(3),N3), (N(4),N4), (N(5),N5)			MAIN	100
	EQUIVALENCE (L(1),I1L), (L(2),I2L), (L(3),I3L), (L(4),I4L),			MAIN	110
	1 (L(5),I5L), (L(6),I6L), (L(7),I7L), (L(8),I8L), (L(9),I9L),			MAIN	120
	2 (L(10),I10L)			MAIN	130
	DATA SS1 /231*0.0Q0/			MAIN	140
	DATA L/10*0/, I/10*0/			MAIN	150
C				MAIN	160
C	DEBUG = .TRUE.			MAIN	170
C	DEBUG = .FALSE.			MAIN	180
	DEBUG = .FALSE.			MAIN	190
	DO 3 K=1,26136			MAIN	200
	3 ZZ(K) = 0.0D0			MAIN	210
	CALL READIN(P)			MAIN	220
C				MAIN	230
C	28-ELEMENTAL (SINGLE-BONDED) DIAGRAMS			MAIN	240
	PRINT 17			MAIN	250
C				MAIN	260
	DO 100 J=1,430			MAIN	270
	IF(DEBUG) PRINT 17			MAIN	280
	17 FORMAT('1')			MAIN	290
	READ (5,1,END=101) S,W,NB,NC,L			MAIN	300
	1 FORMAT(2F10.0,12I2)			MAIN	310
	PRINT 2, J, S, W, NB, NC, L			MAIN	320
	2 FORMAT(I4,2F16.1,2I6,3X,10I3)			MAIN	330
	IF(S .EQ. 0.0D0) GO TO 789			MAIN	340
C				MAIN	350
	INLSUM = 0			MAIN	360
	DO 15 M=1,NB			MAIN	370
	INLSUM = INLSUM + L(M)			MAIN	380
	15 CONTINUE			MAIN	390
C	MOW CHECK ON NC 1"S IN JAO			MAIN	400
C				MAIN	410
	READ 5,JAO			MAIN	420
	5 FORMAT(10I2)			MAIN	430
C	IF(DEBUG) PRINT 6, (JAO(M),M=1,NC)			MAIN	440
	PRINT 6, (JAO(M),M=1,NC)			MAIN	450

6	FORMAT('0 JAO: ',10I4)	MAIN 460
	JAOSUM = 0	MAIN 470
	DO 16 M=1,NC	MAIN 480
	JAOSUM = JAOSUM + JAO(M)	MAIN 490
16	CONTINUE	MAIN 500
C	IF(DEBUG) PRINT 7, JAOSUM	MAIN 510
	PRINT 7, JAOSUM	MAIN 520
	7 FORMAT(' JAO_SUM IS ',I5)	MAIN 530
C		MAIN 540
C	ASSUME JAOSUM > 0	MAIN 550
	DO 18 NNN=1,JAOSUM	MAIN 560
	READ 5, (NP(JJ,NNN),JJ=1,5)	MAIN 570
C	IF(DEBUG) PRINT 8, NNN, (NP(JJ,NNN),JJ=1,5)	MAIN 580
	PRINT 8, NNN, (NP(JJ,NNN),JJ=1,5)	MAIN 590
18	CONTINUE	MAIN 600
	8 FORMAT(I5,5I3)	MAIN 610
C		MAIN 620
C		MAIN 630
C		MAIN 640
C		MAIN 650
	IIT = 10 - INLSUM	MAIN 660
	I1T = IIT + I1L	MAIN 670
	I2T = IIT + I2L	MAIN 680
	I3T = IIT + I3L	MAIN 690
	I4T = IIT + I4L	MAIN 700
	I5T = IIT + I5L	MAIN 710
	I6T = IIT + I6L	MAIN 720
	I7T = IIT + I7L	MAIN 730
	I8T = IIT + I8L	MAIN 740
	I9T = IIT + I9L	MAIN 750
	I10T = IIT + I10L	MAIN 760
10	FORMAT('0 IIT=',I5,5X,'I1T,...I10T=',10I5)	MAIN 770
	IF(DEBUG)	MAIN 780
	*PRINT 10, IIT, I1T,I2T,I3T,I4T,I5T,I6T,I7T,I8T,I9T,I10T	MAIN 790
C		MAIN 800
	DO 90 I1=I1L, I1T	MAIN 810
	I(1)=I1	MAIN 820
	IF(NB .EQ. 1) GO TO 999	MAIN 830
	DO 88 I2=I2L, I2T	MAIN 840
	J2 = I2 + I1	MAIN 850
	IF(J2 .GT. 10) GO TO 90	MAIN 860
	I(2) = I2	MAIN 870
	IF(NB .EQ. 2) GO TO 999	MAIN 880
	DO 86 I3=I3L, I3T	MAIN 890
	J3 = J2 + I3	MAIN 900

IF(J3 .GT. 10) GO TO 88	MAIN 910
I(3) = I3	MAIN 920
IF(NB .EQ. 3) GO TO 999	MAIN 930
DO 84 I4=I4L, I4T	MAIN 940
J4 = J3 + I4	MAIN 950
IF(J4 .GT. 10) GO TO 86	MAIN 960
I(4) = I4	MAIN 970
IF(NB .EQ. 4) GO TO 999	MAIN 980
DO 82 I5=I5L, I5T	MAIN 990
J5 = J4 + I5	MAIN1000
IF(J5 .GT. 10) GO TO 84	MAIN1010
I(5) = I5	MAIN1020
IF(NB .EQ. 5) GO TO 999	MAIN1030
DO 80 I6=I6L, I6T	MAIN1040
J6 = J5 + I6	MAIN1050
IF(J6 .GT. 10) GO TO 82	MAIN1060
I(6) = I6	MAIN1070
IF(NB .EQ. 6) GO TO 999	MAIN1080
DO 78 I7=I7L, I7T	MAIN1090
J7 = J6 + I7	MAIN1100
IF(J7 .GT. 10) GO TO 80	MAIN1110
I(7) = I7	MAIN1120
IF(NB .EQ. 7) GO TO 999	MAIN1130
DO 76 I8=I8L, I8T	MAIN1140
J8=J7+I8	MAIN1150
IF(J8 .GT. 10) GO TO 78	MAIN1160
I(8) = I8	MAIN1170
IF(NB .EQ. 8) GO TO 999	MAIN1180
DO 74 I9=I9L, I9T	MAIN1190
J9 = J8 + I9	MAIN1200
IF(J9 .GT. 10) GO TO 76	MAIN1210
I(9) = I9	MAIN1220
IF(NB .EQ. 9) GO TO 999	MAIN1230
DO 72 I10=I10L, I10T	MAIN1240
J10 = J9 + I10	MAIN1250
IF(J10 .GT. 10) GO TO 74	MAIN1260
I(10) = I10	MAIN1270
	MAIN1280
	MAIN1290
	MAIN1300
	MAIN1310
	MAIN1320
	MAIN1330
	MAIN1340
	MAIN1350

C	
C	
C	
C	
C	
999	F = S
	IF(DEBUG)
	*PRINT 12, I1, I2, I3, I4, I5, I6, I7, I8, I9, I10

12	FORMAT('O I1,...,I10= ',10I5)	MAIN1360
	DO 20 K=2,21	MAIN1370
20	S1(K) = 0.0D0	MAIN1380
	S1(1) = 1.0D0	MAIN1390
	NS1 = 1	MAIN1400
	NNN=0	MAIN1410
	DO 30 II=1,NC	MAIN1420
	IAO = JAO(II)	MAIN1430
	DO 29 III=1,5	MAIN1440
29	N(III)=0	MAIN1450
	DO 27 III = 1, IAO	MAIN1460
	NNN=NNN+1	MAIN1470
	DO 26 JJ=1,5	MAIN1480
	KK=NP(JJ,NNN)	MAIN1490
	IF(KK .LE.0) GO TO 27	MAIN1500
	N(III) = N(III) + I(KK)	MAIN1510
26	CONTINUE	MAIN1520
27	CONTINUE	MAIN1530
C		MAIN1540
C	NOW ORDER THE N(I) AND MULT S1 * P(N, N1+1, N2+1, N3+1)	MAIN1550
C		MAIN1560
C		MAIN1570
	DO 35 I=1,4	MAIN1580
	IS=IN+1	MAIN1590
	DO 35 JN=IS,5	MAIN1600
	IF(N(IN) .LE. N(JN)) GO TO 35	MAIN1610
	NSAVE = N(IN)	MAIN1620
	N(IN) = N(JN)	MAIN1630
	N(JN) = NSAVE	MAIN1640
35	CONTINUE	MAIN1650
	IF(DEBUG) PRINT 11, N	MAIN1660
11	FORMAT(' SORT N IS ',5I5)	MAIN1670
	N11 = N1+1	MAIN1680
	N21 = N2+1	MAIN1690
	N31 = N3+1	MAIN1700
	N41 = N4+1	MAIN1710
	N51 = N5+1	MAIN1720
C		MAIN1730
	NN1 = N1 + N2 + N3 + 1 + N4 + N5	MAIN1740
	CALL POLYMT(P(1,N11, N21, N31, N41, N51), NN1, S1, NS1, S1)	MAIN1750
	NS1 = NS1+NN1-1	MAIN1760
30	CONTINUE	MAIN1770
C		MAIN1780
C		MAIN1790
C		MAIN1800

C		MAIN1810
C		MAIN1820
	KK=0	MAIN1830
	F=S	MAIN1840
	DO 40 K=1,NB	MAIN1850
	FACT = 1.0D0	MAIN1860
	IFK = I(K)	MAIN1870
	DO 28 IFF=1,IFK	MAIN1880
28	FACT = FACT * IFF	MAIN1890
	F = F * FACT	MAIN1900
	IF(DEBUG)	MAIN1910
	*PRINT 9, NB,NC,I, F	MAIN1920
	9 FORMAT(' FACT:',2I6,10I3,1PG20.12)	MAIN1930
40	KK = KK + I(K)	MAIN1940
	IF(KK .GT. 0) GO TO 49	MAIN1950
	PRINT 13, I	MAIN1960
13	FORMAT('1****ERROR KK=0 AND I=',10I5)	MAIN1970
	STOP	MAIN1980
C		MAIN1990
49	CONTINUE	MAIN2000
	KZ=1	MAIN2010
	DO 50 K=1,21	MAIN2020
	SS1(K,KK) = SS1(K,KK) + W*S1(K)/F	MAIN2030
	IF(SS1(K,KK) .NE. 0.0D0) KZ=K	MAIN2040
50	CONTINUE	MAIN2050
C		MAIN2060
C		MAIN2070
C		MAIN2080
C	4 FORMAT(' KK=',I5,1P5G20.12,/, (1P6G20.12))	MAIN2090
C	IF(DEBUG) PRINT 4, KK, (SS1(K,KK),K=1,KZ)	MAIN2100
	PRINT 4, KK, (SS1(K,KK),K=1,KZ)	MAIN2110
	4 FORMAT(' KK=',I5,/, (1P5G26.16))	MAIN2120
60	CONTINUE	MAIN2130
	GO TO (90, 88, 86, 84, 82, 80, 78, 76, 74, 72), NB	MAIN2140
C		MAIN2150
72	CONTINUE	MAIN2160
74	CONTINUE	MAIN2170
76	CONTINUE	MAIN2180
78	CONTINUE	MAIN2190
80	CONTINUE	MAIN2200
82	CONTINUE	MAIN2210
84	CONTINUE	MAIN2220
86	CONTINUE	MAIN2230
88	CONTINUE	MAIN2240
90	CONTINUE	MAIN2250

100	CONTINUE	MAIN2260
101	CONTINUE	MAIN2270
	DO 954 KK=1,11	MAIN2280
	PRINT 4, KK, (SS1(K, KK), K=1, 21)	MAIN2290
	PUNCH 25, (SS1(K, KK), K=2, 21)	MAIN2300
25	FORMAT(1P3G26.16)	MAIN2310
954	CONTINUE	MAIN2320
789	CONTINUE	MAIN2330
	STOP	MAIN2340
	END	MAIN2350

	SUBROUTINE READIN (P)	READ 10
	IMPLICIT REAL*16(A-H,O-Z)	READ 20
C		READ 30
	DIMENSION P(11,3,3,4,6,11), IP(5)	READ 40
	EQUIVALENCE (IP(1),N), (IP(2),L), (IP(3),K), (IP(4),J), (IP(5),I)	READ 50
C		READ 60
	PRINT 1	READ 70
	1 FORMAT('1 READIN P(M,N,L,K,J,I),M=2,11)',//)	READ 80
	DO 100 IR=1,100	READ 90
	READ (9,4) IP	READ 100
	4 FORMAT(5I3)	READ 110
	IF(N .EQ. 0) GO TO 90	READ 120
	READ(9,5) (P(M,N,L,K,J,I),M=2,11)	READ 130
	PRINT 6, N, L, K, J, I, (P(M,N,L,K,J,I),M=2,11)	READ 140
	6 FORMAT('0',5I5,5F13.2,/, (25X,5F13.2))	READ 150
100	CONTINUE	READ 160
	IR=101	READ 170
C		READ 180
	90 CONTINUE	READ 190
	IR=IR-1	READ 200
	PRINT 3, IR	READ 210
	3 FORMAT('0 ',15,' CARDS WERE READIN INTO POLY')	READ 220
	5 FORMAT(10F8.0)	READ 230
	PRINT 2	READ 240
	2 FORMAT('1')	READ 250
	RETURN	READ 260
	END	READ 270

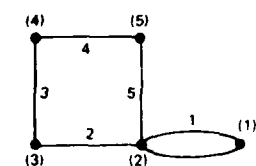
SUBROUTINE POLYMT(P, NP, S, NS, A)	POLY 10
IMPLICIT REAL*16(A-H,O-Z)	POLY 20
DIMENSION P(NP), S(NS), A(21), B(21)	POLY 30
COMMON DEBUG	POLY 40
LOGICAL DEBUG	POLY 50
C	POLY 60
C DEBUG = .TRUE.	POLY 70
C DEBUG = .FALSE.	POLY 80
IF(DEBUG) PRINT 1, NP, (P(I),I=1,11)	POLY 90
IF(DEBUG) PRINT 2, NS, (S(I),I=1,21)	POLY 100
1 FORMAT(' INPUT P POLY NP=',I5, '///,(1P5G20.12))	POLY 110
2 FORMAT(' INPUT S POLY NS=',I5, '///,(1P5G20.12))	POLY 120
3 FORMAT(' OUTPUT THE B POLY'///,(1P5G20.12))	POLY 130
C	POLY 140
DO 10 I=1,21	POLY 150
10 B(I) = 0.0D0	POLY 160
C ASSUME NP .GE. 2	POLY 170
IF(NS .GT. 1) GO TO 20	POLY 180
C SPECIAL FOR NS=1	POLY 190
DO 15 L=1,NP	POLY 200
15 B(L) = S(1) * P(L)	POLY 210
C	POLY 220
C GENERAL RETURN	POLY 230
C	POLY 240
99 CONTINUE	POLY 250
IF(DEBUG) PRINT 3, B	POLY 260
DO 100 L=1,21	POLY 270
A(L) = B(L)	POLY 280
100 CONTINUE	POLY 290
RETURN	POLY 300
C	POLY 310
C	POLY 320
20 CONTINUE	POLY 330
IF(NP .GT. NS) GO TO 40	POLY 340
C FOR NP .LE. NS	POLY 350
NP1 = NP-1	POLY 360
DO 30 L=1,NP1	POLY 370
LP1 = L+1	POLY 380
DO 30 I=1,L	POLY 390
B(L) = B(L) + P(I) * S(LP1-I)	POLY 400
30 CONTINUE	POLY 410
C	POLY 420
DO 33 L=NP,NS	POLY 430
LP1 = L+1	POLY 440
DO 33 I=1,NP	POLY 450

```

      B(L) = B(L) + P(I) * S(LP1-I)
33 CONTINUE
C
      NPNS = NP+ NS
      NS1 = NS+1
      N2 = NPNS - 1
      DO 36 L=NS1, N2
      LNS = L - NS
      I1 = NPNS - L
      DO 36 I=1,I1
      B(L) = B(L) + P(LNS+I) * S(NS1 - I)
36 CONTINUE
      GO TO 99
C
C
C      NP .GT. NS
40 CONTINUE
      NS1 = NS-1
      DO 50 L=1,NS1
      LP1 = L+1
      DO 50 I=1,L
      B(L) = B(L) + S(I) * P(LP1 - I)
50 CONTINUE
C
      DO 53 L=NS, NP
      LP1 = L+1
      DO 53 I=1,NS
      B(L) = B(L) + S(I) * P(LP1 - I)
53 CONTINUE
C
      NP1 = NP+1
      NPNS = NS + NP
      N2 = NPNS - 1
      DO 56 L=NP1, N2
      LNS = NPNS - L
      NPL = L-NP
      DO 56 I=1,LNS
      B(L) = B(L) + S(NPL+I) * P(NP1 - I)
56 CONTINUE
      GO TO 99
      END

```

POLY 460
 POLY 470
 POLY 480
 POLY 490
 POLY 500
 POLY 510
 POLY 520
 POLY 530
 POLY 540
 POLY 550
 POLY 560
 POLY 570
 POLY 580
 POLY 590
 POLY 600
 POLY 610
 POLY 620
 POLY 630
 POLY 640
 POLY 650
 POLY 660
 POLY 670
 POLY 680
 POLY 690
 POLY 700
 POLY 710
 POLY 720
 POLY 730
 POLY 740
 POLY 750
 POLY 760
 POLY 770
 POLY 780
 POLY 790
 POLY 800
 POLY 810
 POLY 820
 POLY 830
 POLY 840
 POLY 850
 POLY 860



(p) labels the vertices

i labels the bond

$$S = 2$$

$$W = \begin{cases} 6480 & \text{for f.c.c.} \\ 540 & \text{for s.c.} \\ 1728 & \text{for b.c.c.} \end{cases}$$

$$NB = 5$$

$$L = (2, 1, 1, 1, 1, 0, 0, 0, 0, 0)$$

$$INSLUM = 6$$

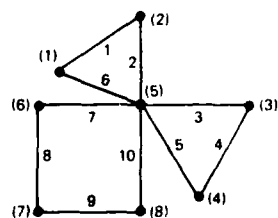
$$NC = 5$$

$$JAO = (1, 2, 1, 1, 1, 0, 0, 0, 0, 0)$$

$$JAOSUM = 6$$

Circle	NNN	NP
(1)	1	1, 0, 0, 0, 0
(2)	2	1, 0, 0, 0, 0
	3	2, 5, 0, 0, 0
(3)	4	2, 3, 0, 0, 0
(4)	5	3, 4, 0, 0, 0
(5)	6	4, 5, 0, 0, 0
	11T =	4
	11T =	6
	12T =	5
	13T =	5
	14T =	5
	15T =	5

Figure A-1—An illustration of the notations used in the main program. (The diagram's symmetry number does not account for the interchangeability of multiple bonds between a connected pair of vertices.)



(p) labels the vertices

i labels the bond

$$S = 16$$

$$W = \begin{cases} 1, 244, 160 & \text{for f.c.c.} \\ 0 & \text{for s.c.} \\ 0 & \text{for b.c.c.} \end{cases}$$

$$NB = 10$$

$$L = (1, 1, 1, 1, 1, 1, 1, 1, 1, 1)$$

$$INSLUM = 10$$

$$NC = 8$$

$$JAO = (1, 1, 1, 1, 3, 1, 1, 1, 0, 0)$$

$$JAOSUM = 10$$

Circle	NNN	NP
(1)	1	1, 6, 0, 0, 0
(2)	2	1, 2, 0, 0, 0
(3)	3	3, 4, 0, 0, 0
(4)	4	4, 5, 0, 0, 0
(5)	5	2, 6, 0, 0, 0
	6	3, 5, 0, 0, 0
	7	5, 6, 0, 0, 0
(6)	8	7, 8, 0, 0, 0
(7)	9	8, 9, 0, 0, 0
(8)	10	9, 10, 0, 0, 0

Figure A-2—An example of the notation used in the main program

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The work reported in TG 1337 was done under Navy Contract N00024-83-C-5301. This work is supported by the Naval Sea Systems Command.

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