Free multiplicities and weak lattice constants

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Lattice constants used in the linked-cluster expansions, called free multiplicities, are given in terms of weak lattice constants for graphs up to nine edges. The procedure of deriving these relations is computerized and can be easily extended to graphs of more edges. The method of single-number representation of graphs has been used in the derivation.

I. INTRODUCTION

In deriving high-temperature series expansions for spin systems, two approaches which are generally used are the finite-cluster method and the linked-cluster expansion method.[1] The finite-cluster method was first suggested by Domb,[2] and had been applied to many systems such as the Heisenberg model,[3–5] the exchange-interaction model,[6,7] etc. The linked-cluster expansion method first applied to spin systems by Englert[8] was then developed by Wortis and co-workers.[9–11] Recently the linked-cluster expansion method has been modified by Wang and Lee.[12] The modified method is very powerful in deriving series expansions even for systems having complicated energy levels and has been applied to many spin systems,[13–16] especially those having crystal fields or multipole exchange interactions.

The lattice constants that occur in the finite-cluster method are weak lattice constants (also called weak embeddings). Extensive tabulations of these constants have been given by Baker *et al.*[17] In the linked-cluster expansion method, the lattice constants used are called free multiplicities.[9] They have not been carefully studied, and published data are rather limited.[18] Since free multiplicities are closely related to weak lattice constants, it is the purpose of this paper to find the expressions of free multiplicities in terms of weak lattice constants. The exploration includes all graphs up to nine edges.

In Sec. II we briefly describe the linked-cluster expansion technique. Methods to evaluate the free multiplicities are also discussed. The procedure for finding the expressions of free multiplicities in terms of weak lattice constants is described in Sec. III. The results for graphs up to nine edges are given in the Appendix. Some conclusions are given in Sec. IV.

II. LINKED-CLUSTER EXPANSION AND FREE MULTIPLICITIES

To formulate the expansion, the system Hamiltonian is separated as $H=H_0+H_1$. The unperturbed term H_0 is the single-ion potential including self-consistent parameters which are used to minimize the free energy. The perturbed term H_1 describes the correlations of the spin fluctuation. The free-energy shift is given by

$$-\beta\Delta F=\sum_{l=2}^{\infty}\frac{(-1)^l}{l!}\int_0^\beta d\tau_1\int_0^\beta d\tau_2\cdots\int_0^\beta d\tau_l\langle T[\hat{H}_1(\tau_1)\hat{H}_1(\tau_2)\cdots\hat{H}_1(\tau_l)]\rangle_c \tag{1}$$

with the Dyson τ-ordering T operating on the interaction representation $\hat{H}_1(\tau)$. The subscript c denotes the cumulant average over H_0.

In terms of standard basis operators,[19,20] the τ integrations are greatly simplified by the permutation symmetry[21] and become trivial in Ising-type systems. The semi-invariants linked by interactions are represented by linear graphs. The corresponding summation of interactions over all lattice sites defines the free multiplicity of the graph.

For a graph g of p vertices, the free multiplicity of g on a lattice L of N sites, denoted $m(g;L)$, is defined as

$$m(g;L)=\frac{1}{N}\sum_{x_1=1}^{N}\cdots\sum_{x_i=1}^{N}\cdots\sum_{x_p=1}^{N}\cdots\prod_{\langle ij\rangle}J(x_i,x_j)\ , \tag{2}$$

where the summations $\sum_{x_i=1}^{N}$ run over all sites of the lattice L, and the product covers all connected pairs of vertices $\langle ij\rangle$ of g. For the nearest-neighbor interaction model, the exchange constants $J(x_i,x_j)$ can be taken as 1 (i.e., the temperature is measured in units of J), if x_i and x_j are nearest-neighbor sites of L. Otherwise, $J(x_i,x_j)=0$.

The evaluation of free multiplicities is one of the important steps in deriving the linked-cluster expansions. The free multiplicities had been calculated by momentum-space interaction. By taking the Fourier transform of the exchange constant, a free multiplicity is then evaluated by integration over the first Brillouin zone in the $\vec{k}$ space.[12,22] For low-order graphs, this calculation can be done manually. This method becomes clumsy and impractical even for graphs of moderate orders.

With the aid of a computer, $m(g;L)$ can be calculated by performing random walks on the lattice L.[23] The number of different walks that have a path isomorphic to g is equal to $m(g;L)$. This is a convenient way to calculate $m(g;L)$. The computation time in this method, however, increases rapidly with the coordination number of L and with the number of vertices of g.

As mentioned in the Introduction, weak lattice constants, to be denoted as $p(g;L)$, are known for most lattices. We find that it is easier to derive $m(g;L)$ from $p(g;L)$. It is our purpose here to find the expressions of $m(g;L)$ in terms of $p(g;L)$.

III. FREE MULTIPLICITIES AND WEAK LATTICE CONSTANTS

In the summations of Eq. (2), the lattice sites $x_1,x_2,\ldots,x_p$ are allowed to be the same; that is, vertices of the graph g which are not joined directly by an edge can be embedded on the same site of the lattice L. [When two vertices joined by an edge are embedded on the same site, it does not contribute to $m(g;L)$ because $J(x_i,x_i)=0$.] If the summations in Eq. (2) are restricted such that $x_1,x_2,\ldots,x_p$ are all different, then the right-hand side of Eq. (2) is equal to $p(g;L)S(g)$, where $p(g;L)$ is the weak lattice constant of g and $S(g)$ is the symmetry number of g.

From the above observation, a free multiplicity $m(g_i;L)$ can be written as

$$m(g_i;L)=\sum_j t_{ij}S(g_j)p(g_j;L)\ , \tag{3}$$

where the summation takes over all graphs g_j which are obtained by bringing some unjoined vertices of g_i into coincidence and then replacing multiple edges by single edges. A graph g_j obtained in this way is called a reduced graph of g_i. The constants t_{ij} are the number of different ways of obtaining the reduced graphs g_j from g_i. If the order (number of vertices) of g_i is low, the coefficients t_{ij} can be obtained by observation.[24] For high-order graphs, the coefficients are difficult to determine manually. We have developed a method to count t_{ij} by a computer.

A brief outline of our procedure is as follows: (i) A given graph g_i is represented numerically by its incidence matrix $A(g_i)$, (ii) all possible methods of bringing unjoined vertices of g_i into coincidence are performed, (iii) for each method of coincidence of vertices a new matrix $A(g_j)$ which represents a graph g_j is obtained, (iv) the graph g_j is identified by the single-number representation of graph, and (v) a count is made of the number of times that a reduced graph g_j is obtained.

The single-number representation of graphs provides a good practical algorithm for the identification of graphs. It has been discussed in detail by the authors[25] and will not be described here. For graphs up to nine edges, only 34 free multiplicities $m(g_i;L)$ need to be calculated (see the Appendix). Free multiplicities of other graphs are products of free multiplicities of these irreducible graphs.[9] We have calculated the coefficients t_{ij} in Eq. (3) for the 34 irreducible graphs. It takes less than 50 sec for a CDC model Cyber-172 computer to determine all the coefficients t_{ij}. The results are shown in the Appendix, in which $m(i)$ and $p(i)$ are, respectively, the free multiplicity and the weak lattice constant of the graph whose identification number is i. We have adopted the graph identification number given by Baker *et al.*[17] The variable L has been omitted for convenience.

IV. CONCLUSION

The linked-cluster expansion method is a powerful approach in deriving series expansions for spin systems, even for those having complicated crystal fields or exchange interactions. It can be used to derive series expansions that are valid not only at high temperature, but also at low temperature[16] (and even at zero temperature[14]). The lattice constants used in the linked-cluster expansion method, called free multiplicities, have not been carefully studied. In this article we have derived the expressions of free multiplicities in terms of the well-studied weak lattice constants. Through these expressions free multiplicities can be obtained easily.

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APPENDIX: RELATIONS BETWEEN FREE MULTIPLICITIES AND WEAK LATTICE CONSTANTS

Listed are the relations between free multiplicities $m(i)$ and weak lattice constants $p(i)$ for irreducible graphs up to nine edges. The graph identification numbers i are adopted from Baker *et al.*[17] We have the following:

$$m(3)=6p(3)\ ,$$

$$m(6)=8p(6)+4p(2)+2p(1)\ ,$$

$$m(12)=10p(12)+10p(7)+30p(3)\ ,$$

$$m(23)=24p(23)\ ,$$

$$m(24)=12p(24)+24p(6)+6p(4)+8p(2)+2p(1)\ ,$$

$$m(29)=12p(29)+24p(26)+12p(13)+36p(11)+48p(6)+6p(5)+12p(4)+24p(3)+12p(2)+2p(1)\ ,$$

$$m(55)=4p(55)+8p(11)+2p(7)+12p(3)\ ,$$

$$m(61)=4p(61)+4p(28)+8p(25)+4p(15)+10p(12)+28p(11)+18p(7)+42p(3)\ ,$$

$$m(76)= 14p(76)+28p(60)+84p(54)+14p(30)+42p(25)+14p(16)+28p(15)+14p(14)$$
$$+70p(12)+112p(11)+84p(7)+126p(3)\ ,$$
$$m(133)=8p(133)+8p(11)+6p(3)\ ,$$
$$m(139)=48p(139)+72p(24)+24p(8)+56p(6)+36p(4)+16p(2)+2p(1)\ ,$$
$$m(141)= 8p(141)+8p(133)+48p(24)+4p(13)+8p(11)+64p(6)+2p(5)+12p(4)+6p(3)+12p(2)+2p(1)\ ,$$
$$m(154)=4p(154)+12p(56)+8p(53)+8p(26)+120p(23)+24p(11)+12p(3)\ ,$$
$$m(155)=2p(155)+4p(55)+4p(53)+4p(28)+4p(25)+24p(23)+32p(11)+6p(7)+24p(3)\ ,$$
$$m(158)= 4p(158)+8p(136)+4p(135)+4p(75)+12p(74)+16p(57)+8p(55)+36p(54)+24p(53)$$
$$+4p(33)+12p(29)+4p(28)+24p(26)+96p(24)+96p(23)+32p(13)+84p(11)+2p(9)$$
$$+24p(8)+4p(7)+128p(6)+10p(5)+42p(4)+36p(3)+20p(2)+2p(1)\ ,$$
$$m(159)= 4p(159)+4p(135)+4p(71)+8p(69)+8p(61)+8p(58)+4p(55)+16p(53)+20p(28)$$
$$+8p(27)+48p(26)+28p(25)+96p(23)+8p(15)+4p(14)+10p(12)+128p(11)+36p(7)+78p(3)\ ,$$
$$m(223)= 16p(223)+32p(161)+32p(160)+96p(140)+96p(139)+16p(108)+32p(70)+64p(69)$$
$$+32p(59)+48p(58)+48p(57)+128p(53)+16p(34)+32p(33)+16p(32)+16p(31)$$
$$+96p(29)+96p(28)+48p(27)+320p(26)+64p(25)+192p(24)+528p(23)+112p(13)$$
$$+464p(11)+8p(10)+16p(9)+48p(8)+64p(7)+264p(6)+32p(5)+72p(4)+168p(3)+28p(2)+2p(1)\ ,$$
$$m(374)=8p(374)+20p(55)+4p(15)+16p(11)+10p(7)+24p(3)\ ,$$
$$m(376)=2p(376)+8p(132)+6p(56)+6p(53)+120p(23)+12p(11)+6p(3)\ ,$$
$$m(377)=12p(377)+12p(53)+72p(23)+24p(11)+12p(3)\ ,$$
$$m(378)=2p(378)+8p(133)+8p(55)+12p(54)+2p(28)+2p(25)+28p(11)+4p(7)+18p(3)\ ,$$
$$m(379)=72p(379)+72p(24)+72p(6)+12p(4)+12p(2)+2p(1)\ ,$$
$$m(384)= 12p(384)+12p(146)+12p(138)+12p(61)+24p(55)+84p(54)+12p(37)+12p(28)$$
$$+24p(25)+36p(15)+10p(12)+84p(11)+46p(7)+66p(3)\ ,$$
$$m(467)= 4p(467)+4p(372)+24p(366)+4p(152)+4p(150)+4p(134)+16p(133)+44p(132)$$
$$+4p(60)+24p(55)+48p(54)+8p(53)+4p(28)+8p(27)+8p(25)+240p(23)+2p(16)$$
$$+4p(15)+72p(11)+14p(7)+36p(3)\ ,$$
$$m(468)=p(468)+2p(372)+2p(370)+2p(155)+2p(152)+2p(151)+2p(138)+4p(136)$$
$$+2p(135)+2p(134)+16p(133)+12p(132)+p(71)+2p(58)+24p(55)+36p(54)$$
$$+18p(53)+8p(28)+6p(27)+16p(26)+12p(25)+144p(23)+4p(15)$$
$$+2p(14)+96p(11)+18p(7)+48p(3)\ ,$$
$$m(469)= 2p(469)+2p(376)+4p(155)+2p(149)+4p(138)+2p(134)+8p(132)+2p(71)+8p(61)$$
$$+6p(56)+16p(55)+24p(54)+14p(53)+12p(28)+4p(27)+26p(25)+120p(23)$$
$$+8p(15)+2p(14)+10p(12)+92p(11)+30p(7)+60p(3)\ ,$$
$$m(470)= 4p(470)+4p(378)+4p(151)+8p(138)+16p(133)+8p(61)+4p(60)+36p(55)$$
$$+48p(54)+2p(30)+8p(28)+28p(25)+2p(16)+12p(15)+4p(14)$$
$$+20p(12)+96p(11)+40p(7)+72p(3)\ ,$$
$$m(473)=6p(473)+6p(372)+24p(141)+24p(133)+12p(132)+18p(74)+12p(57)+36p(54)$$
$$+12p(53)+156p(24)+96p(23)+24p(13)+48p(11)+24p(8)+144p(6)+6p(5)$$
$$+42p(4)+18p(3)+20p(2)+2p(1)\ ,$$

$$m(475)=6p(475)+12p(154)+6p(149)+12p(135)+24p(56)+12p(55)+48p(53)+12p(28)+24p(26)+264p(23)+96p(11)+6p(7)+36p(3)\ ,$$

$$m(476)=8p(476)+8p(155)+16p(140)+8p(65)+8p(61)+8p(55)+24p(53)+32p(28)+16p(25)+96p(23)+8p(15)+10p(12)+104p(11)+26p(7)+54p(3)\ ,$$

$$m(490)=12p(490)+12p(461)+48p(381)+12p(371)+24p(359)+12p(218)+24p(158)+12p(154)+12p(148)+72p(136)+24p(135)+12p(134)+48p(132)+24p(75)+48p(74)+84p(57)+36p(56)+48p(55)+168p(54)+144p(53)+24p(33)+12p(32)+36p(29)+24p(28)+24p(27)+96p(26)+12p(25)+288p(24)+696p(23)+108p(13)+300p(11)+12p(9)+48p(8)+24p(7)+288p(6)+26p(5)+72p(4)+96p(3)+28p(2)+2p(1)\ ,$$

$$m(530)=4p(530)+8p(482)+24p(481)+8p(478)+4p(463)+4p(371)+16p(369)+8p(368)+144p(367)+24p(359)+4p(222)+4p(221)+8p(157)+8p(155)+12p(140)+36p(138)+12p(134)+32p(132)+4p(105)+14p(76)+4p(73)+8p(72)+12p(71)+4p(67)+8p(65)+4p(63)+36p(61)+52p(60)+96p(55)+324p(54)+44p(53)+4p(39)+24p(37)+4p(36)+22p(30)+52p(28)+24p(27)+138p(25)+288p(23)+18p(16)+96p(15)+30p(14)+90p(12)+364p(11)+156p(7)+186p(3)\ ,$$

$$m(531)=2p(531)+4p(484)+4p(471)+2p(463)+2p(461)+4p(371)+4p(369)+8p(368)+12p(359)+4p(221)+2p(220)+2p(215)+4p(211)+8p(159)+4p(157)+4p(156)+8p(155)+4p(154)+2p(148)+12p(146)+12p(140)+12p(138)+8p(137)+20p(136)+16p(135)+12p(134)+40p(132)+6p(73)+4p(72)+14p(71)+4p(70)+16p(69)+2p(66)+8p(65)+8p(63)+32p(61)+24p(60)+20p(58)+12p(56)+64p(55)+192p(54)+96p(53)+2p(40)+12p(37)+6p(30)+80p(28)+34p(27)+104p(26)+106p(25)+504p(23)+10p(16)+52p(15)+16p(14)+40p(12)+404p(11)+108p(7)+162p(3)\ ,$$

$$m(659)=18p(659)+36p(488)+36p(487)+108p(384)+108p(383)+108p(382)+144p(381)+72p(380)+288p(360)+18p(224)+36p(213)+36p(212)+72p(211)+36p(210)+36p(162)+54p(157)+54p(156)+216p(146)+108p(145)+144p(138)+108p(137)+216p(136)+144p(134)+396p(132)+18p(107)+18p(106)+36p(105)+18p(104)+126p(76)+54p(73)+54p(72)+108p(71)+144p(61)+396p(60)+72p(58)+396p(55)+1656p(54)+324p(53)+18p(41)+36p(40)+36p(39)+18p(38)+108p(37)+36p(36)+18p(35)+144p(30)+288p(28)+216p(27)+288p(26)+666p(25)+1872p(23)+144p(16)+360p(15)+180p(14)+360p(12)+1584p(11)+522p(7)+510p(3)\ .$$

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