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Lattice constant systems and some of their properties†

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Abstract. Lattice constants are defined in a general way such that weak lattice constants, strong lattice constants, free multiplicities and coincidable occurrence factors are cases of the generalised lattice constants. A general method to express a lattice constant of one system as a linear combination of lattice constants of another system is described. Some properties of the conversion matrices are discussed. A systematic method to express the lattice constant of a reducible graph in terms of lattice constants of irreducible graphs is also studied.

1. Introduction

In perturbation expansions of thermodynamic properties of lattice models it is most convenient to represent the various terms in the expansions by linear graphs (Domb 1974). The number of terms in an expansion which are represented by a graph g is usually called the lattice constant of the graph g on the lattice. Associated with different types of series expansions are several lattice constant systems. Well known examples are the weak lattice constants used in the high-temperature series expansion and the strong lattice constants occurring in the low-temperature series expansion (Domb 1960). Other lattice constant systems studied are the free multiplicities (Wortis 1974) and the coincidable occurrence factors (Chen and Lee 1980).

The lattice constants mentioned above are extensive in the sense that if g is a connected graph and if all vertices of the lattice G are equivalent then the lattice constants $L(g; G)$ are proportional to the number of vertices of G. There are lattice constants which are not extensive, such as the weak full perimeter lattice constant and the strong full perimeter lattice constant (Essam 1967). Only extensive lattice constant system will be considered in this article. We will define lattice constants in a general way such that all extensive lattice constant systems studied before are cases of the generalised lattice constants.

All extensive lattice constant systems are linearly related and are derivable from one another. The conversion matrix that transforms the set of strong lattice constants to that of weak lattice constants was studied by Sykes *et al* (1966); the relation of the free multiplicities to the weak lattice constants was discussed by Wortis (1974); and the connection between the coincidable occurrence factors and the weak lattice constants was considered by Chen and Lee (1980). In this article a general method to express a lattice constant of any system as a linear combination of lattice constants of another system is studied.

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In any lattice constant system the lattice constant of a reducible graph can be expressed as a function of lattice constants of irreducible graphs. The reduction of disconnected lattice constants to connected lattice constants, and of articulated lattice constants to star lattice constants, had been considered by Domb (1960, 1974) and Sykes *et al* (1966) for the weak lattice constant system. We present in this article a systematic method to obtain the reduction of lattice constants in any lattice constant system.

The lattice constants $L_\alpha(g; G)$ are defined in § 2. We only consider the case that g are unrooted graphs. The method to obtain the expression of a lattice constant as a linear combination of lattice constants of another system is studied in § 3. The method to express the lattice constant of a reducible graph in terms of lattice constants of irreducible graphs is studied in § 4. Conclusions are given in § 5.

2. Lattice constants

Consider a graph (or lattice) G of N vertices and a graph g of p vertices. The incidence matrix A (for graph terminology see Domb (1974)) of the graph G is defined as

$$A_{ij} = 1 \qquad \text{if } i \neq j \text{ and vertices } i \text{ and } j \text{ are connected,}$$
$$= 0 \qquad \text{otherwise.} \tag{1}$$

A lattice constant of g on G is the number of ways to select p vertices from G according to the connectivity of g. It can be defined generally as

$$L_\alpha(g; G) = \sum_{x_1=1}^{N} \dots \sum_{x_i=1}^{N} \dots \sum_{x_p=1}^{N} \prod_{\langle ij \rangle}^{(c)} C_\alpha(x_i, x_j) \prod_{\langle mn \rangle}^{(d)} D_\alpha(x_m, x_n), \tag{2}$$

where the subscript α refers to different lattice constant systems. The summation $\Sigma_{x_i=1}^{N}$ indicates that we may choose any vertex of G as the ith vertex of g. The first product $\Pi^{(c)}$ covers all connected pairs of vertices of g, and the second product $\Pi^{(d)}$ covers all disconnected pairs of vertices.

The function $C_\alpha(x_i, x_j)$ describes the requirement that a pair of vertices x_i and x_j of G can be selected as a connected pair of vertices i and j of g, while $D_\alpha(x_m, x_n)$ describes the condition that two vertices x_m and x_n of G can be selected as a disconnected pair of vertices m and n of the graph g. The functions C_α and D_α have only two values 0 and 1. All possible forms of C_α and D_α are shown in table 1. Since $f_7(x_i, x_j)(=\delta_{x_ix_j})$ and $f_8(x_i, x_j)(=0)$ give only trivial results, they will not be considered further.

As $L_\alpha(g; G)$ are extensive, C_α has only two alternatives, f_5 and f_6. D_α is less restricted, and can be f_1, f_2, f_3 or f_4. From the two C_α functions and the four D_α

Table 1. Possible functions of $C_\alpha(x_i, x_j)$ and $D_\alpha(x_i, x_j)$. Since either x_i and x_j can be connected or disconnected, or $x_i = x_j$, eight different functions can be defined. $A_{x_ix_j}$ is defined by (1) and $\delta_{x_ix_j}$ is the Kronecker delta.

$f_1(x_i, x_j) \equiv 1$	$f_5(x_i, x_j) \equiv A_{x_ix_j} + \delta_{x_ix_j}$
$f_2(x_i, x_j) \equiv 1 - \delta_{x_ix_j}$	$f_6(x_i, x_j) \equiv A_{x_ix_j}$
$f_3(x_i, x_j) \equiv 1 - A_{x_ix_j}$	$f_7(x_i, x_j) \equiv \delta_{x_ix_j}$
$f_4(x_i, x_j) \equiv 1 - A_{x_ix_j} - \delta_{x_ix_j}$	$f_8(x_i, x_j) \equiv 0$

functions, eight different lattice constant systems can be constructed. They are shown in table 2. Probably all non-trivial extensive lattice constant systems are included in this table. Among the eight systems only four of them (L_1, L_3, L_4 and L_5) have been studied. The weak lattice constant of g on G, usually denoted as $(g; G)$, is related to L_3 by $(g; G) = L_3(g; G)/S(g)$, where $S(g)$ is the symmetry number of the graph g. The strong lattice constant of g, denoted as $[g, G]$, is given by $[g; G] = L_4(g, G)/S(g)$. Two other lattice constant systems studied before are the free multiplicity $m(g, G) = L_1(g; G)$, and the coincidable occurrence factor $C(g; G) = L_5(g; G)$.

Table 2. Lattice constant systems $L_\alpha(g; G)$ defined by (2).

Lattice constants	$C_\alpha(x_i, x_j)$	$D_\alpha(x_i, x_j)$
L_1	$A_{x_ix_j}$	1
L_2	$A_{x_ix_j}$	$1 - A_{x_ix_j}$
L_3	$A_{x_ix_j}$	$1 - \delta_{x_ix_j}$
L_4	$A_{x_ix_j}$	$1 - A_{x_ix_j} - \delta_{x_ix_j}$
L_5	$A_{x_ix_j} + \delta_{x_ix_j}$	1
L_6	$A_{x_ix_j} + \delta_{x_ix_j}$	$1 - A_{x_ix_j}$
L_7	$A_{x_ix_j} + \delta_{x_ix_j}$	$1 - \delta_{x_ix_j}$
L_8	$A_{x_ix_j} + \delta_{x_ix_j}$	$1 - A_{x_ix_j} - \delta_{x_ix_j}$

3. Linear relations between lattice constant systems

All lattice constant systems listed in table 2 are linearly related. As mentioned in § 1, methods to find the expressions of L_3 in terms of L_1, L_4 and L_5, respectively (and their inversions), had been studied. We will describe below a general method to express an arbitrary lattice constant L_α as a linear combination of lattice constants of another system L_β.

We first express $C_\alpha(x_i, x_j)$ and $D_\alpha(x_i, x_j)$ in terms of $C_\beta(x_i, x_j)$, $D_\beta(x_i, x_j)$ and $\delta_{x_ix_j}$. The general forms are

$$C_\alpha(x_i, x_j) = C_\beta(x_i, x_j) + q_{\alpha\beta}\delta_{x_ix_j} \tag{3a}$$

and

$$D_\alpha(x_i, x_j) = D_\beta(x_i, x_j) + r_{\alpha\beta}C_\beta(x_i, x_j) + s_{\alpha\beta}\delta_{x_ix_j} \tag{3b}$$

where $q_{\alpha\beta} = 0, \pm 1$; $r_{\alpha\beta} = 0, \pm 1$ and $s_{\alpha\beta} = 0, \pm 1, \pm 2$. The specific forms of (3a) and (3b) for all possible values of α and β are given in table 3. The lattice constant $L_\alpha(g; G)$ of (2) is then rewritten as

$$L_\alpha(g; G) = \sum_{\{x\}} \prod^{(c)} (C_\beta + q\delta) \prod^{(d)} (D_\beta + rC_\beta + s\delta), \tag{4}$$

where $\Sigma_{\{x\}}$ stands for the p-tuple sum, and the arguments x_i and x_j of the functions $C_\beta(x_i, x_j)$, $D_\beta(x_i, x_j)$ and $\delta_{x_ix_j}$ have been dropped for simplicity. The indices α and β in the coefficients q, r and s are also omitted.

For a graph of p vertices and l edges there are in total $p(p-1)/2$ factors in the double products of (4). If there are n_c terms ($n_c = 1$ or 2) in each factor associated

Table 3. Expressing $C_\alpha(x_i, x_j)$ and $D_\alpha(x_i, x_j)$ as linear combinations of $C_\beta(x_i, x_j)$, $D_\beta(x_i, x_j)$ and $\delta_{x_i x_j}$ (see (3)). The arguments are omitted for simplicity.

β	1	2	3	4	5	6	7	8
$C_1=$	C	C	C	C	$C-\delta$	$C-\delta$	$C-\delta$	$C-\delta$
$D_1=$	D	$D+C$	$D+\delta$	$D+C+\delta$	D	$D+C-\delta$	$D+\delta$	$D+C$
$C_2=$	C	C	C	C	$C-\delta$	$C-\delta$	$C-\delta$	$C-\delta$
$D_2=$	$D-C$	D	$D-C+\delta$	$D+\delta$	$D-C+\delta$	D	$D-C+2\delta$	$D+\delta$
$C_3=$	C	C	C	C	$C-\delta$	$C-\delta$	$C-\delta$	$C-\delta$
$D_3=$	$D-\delta$	$D+C-\delta$	D	$D+C$	$D-\delta$	$D+C-2\delta$	D	$D+C-\delta$
$C_4=$	C	C	C	C	$C-\delta$	$C-\delta$	$C-\delta$	$C-\delta$
$D_4=$	$D-C-\delta$	$D-\delta$	$D-C$	D	$D-C$	$D-\delta$	$D-C+\delta$	D
$C_5=$	$C+\delta$	$C+\delta$	$C+\delta$	$C+\delta$	C	C	C	C
$D_5=$	D	$D+C$	$D+\delta$	$D+C+\delta$	D	$D+C-\delta$	$D+\delta$	$D+C$
$C_6=$	$C+\delta$	$C+\delta$	$C+\delta$	$C+\delta$	C	C	C	C
$D_6=$	$D-C$	D	$D-C+\delta$	$D+\delta$	$D-C+\delta$	D	$D-C+2\delta$	$D+\delta$
$C_7=$	$C+\delta$	$C+\delta$	$C+\delta$	$C+\delta$	C	C	C	C
$D_7=$	$D-\delta$	$D+C-\delta$	D	$D+C$	$D-\delta$	$D+C-2\delta$	D	$D+C-\delta$
$C_8=$	$C+\delta$	$C+\delta$	$C+\delta$	$D+\delta$	C	C	C	C
$D_8=$	$D-C-\delta$	$D-\delta$	$D-C$	D	$D-C$	$D-\delta$	$D-C+\delta$	D

with a connected pair of vertices, and n_d terms ($n_d = 1, 2$, or 3) with a disconnected pair of vertices, there will be a number $N_t = (n_d)^{p(p-1)/2}(n_c/n_d)^l$ of terms in the expansion of (4). Each term will represent a lattice constant $L_\beta(g'; G)$ of a certain graph g'. Of course there are also $p(p-1)/2$ factors in each term $L_\beta(g'; G)$. Each factor describes the connectivity of a pair of vertices of the graph g'. A factor $C_\beta(x_i, x_j)$ indicates that the vertices i and j of the graph g' are connected; a factor $D_\beta(x_k, x_l)$ shows that the vertices k and l of the graph g' are disconnected; and a factor $\delta_{x_m x_n}$ means that the vertices m and n are to be merged (to be glued together). When some vertices are merged, the graph g' will contain less than p vertices.

It should be noted that some of the N_t terms in the expansion of (4) may vanish. For example consider the following case:

$$\sum_{x_1}\cdots\sum_{x_i}\sum_{x_j}\sum_{x_k}\cdots D_\beta(x_i, x_j)\delta_{x_i x_k}\delta_{x_j x_k}\cdots = \sum_{x_i}\cdots\sum_{x_k}\cdots D_\beta(x_k, x_k)\ldots. \tag{5}$$

Since $D_\beta(x_k, x_k) = 0$, or 1, the term given by (5) vanishes if $D_\beta(x_k, x_k) = 0$. On the other hand the factor $D_\beta(x_k, x_k)$ can be dropped if it equals 1. For the purpose of determining whether a term vanishes or not, it is most convenient to represent diagrammatically the factor $C_\beta(x_i, x_j)$ by a full line connecting vertices i and j, the factor $D_\beta(x_k, x_l)$ by a broken line connecting vertices k and l, and the factor $\delta_{x_m x_n}$ by a wavy line joining vertices m and n. If $C_\beta(x, x) = 0$, a term vanishes when two vertices connected directly by a full line are also connected indirectly by wavy lines. Similarly, if $D_\beta(x, x) = 0$, a term vanishes when two vertices connected directly by a broken line are also connected indirectly by wavy lines.

When vertices connected by wavy lines (δ functions) are merged, the graph g' may contain multiple edges. That is, a pair of vertices x_i and x_j may be connected by several full lines (C functions) and broken lines (D functions). Mathematically this means that the term contains the factors $C^n_\beta(x_i, x_j)D^m_\beta(x_i, x_j)$. The multiple edges can then be reduced to single edges by the properties $C_\beta^n = C_\beta$, $D_\beta^m = D_\beta$ and

$$C_\beta(x_i, x_j)D_\beta(x_i, x_j) = C_\beta(x_i, x_j) \qquad \text{for } \beta = 1, 3, 5 \tag{6a}$$

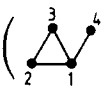
$$= 0 \qquad \text{for } \beta = 2, 4, 8, \tag{6b}$$

$$= \delta_{x_i x_j} \qquad \text{for } \beta = 6, \tag{6c}$$

$$= C_\beta(x_i, x_j) - \delta_{x_i x_j} \qquad \text{for } \beta = 7. \tag{6d}$$

For $\beta = 6$ and 7, δ functions are involved. The vertices x_i and x_j should be merged, and the same procedure should be repeated.

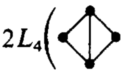
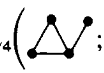
To illustrate the method described above, we consider the following example which expresses $L_1(g; G)$ in terms of $L_4(g'; G)$:

$L_1\Big($ 

$; G\Big)$

$$= \sum_{\{x\}} C_1(12)C_1(13)C_1(14)C_1(23)D_1(24)D_1(34) \tag{7a}$$

$$= \sum_{\{x\}} C_4(12)C_4(13)C_4(14)C_4(23)\times[C_4(24)C_4(34) + C_4(24)D_4(34) + C_4(24)\delta(34) + D_4(24)C_4(34) + D_4(24)D_4(34) + D_4(24)\delta(34) + \delta(24)C_4(34) + \delta(24)D_4(34) + \delta(24)\delta(34)] \tag{7b}$$

$= L_4\Big($  $; G\Big) + 2L_4\Big($  $: G\Big) + L_4\Big($  $; G\Big) + 2L_4\Big($  $; G\Big).$ (7c)

Here the arguments (ij) are shorthand notations of (x_i, x_j).

The relations $C_1 = C_4$ and $D_1 = C_4 + D_4 + \delta$ (see table 3) have been used to obtain (7*b*). The first term in (7*b*) gives the first term in (7*c*). The second and fourth terms in (7*b*) are equal and give the second term in (7*c*). The fifth term in (7*b*) vanishes because $C_4(x, x) = 0$; the sixth and eighth terms vanish because $C_4D_4 = 0$. Finally, the rest of the terms in (7*b*) contribute to the fourth term in (7*c*).

In general we can express the linear relations between two systems of lattice constant in the form

$$L_\alpha(g_i, G) = \sum_j t_{ij}^{\alpha\beta} L_\beta(g_j; G). \tag{8}$$

From the procedure described above some properties of the coefficients $t_{ij}^{\alpha\beta}$ can be observed easily:

(i) the diagonal element $t_{ii}^{\alpha\beta} = 1$,

(ii) $t_{ij}^{\alpha\beta} = 0$ if g_j has more vertices than g_i,

(iii) $t_{ij}^{\alpha\beta} = 0$ if g_j and g_i have the same number of vertices and g_i is not a subgraph of g_j.

Property (iii) comes from the fact that if g_j and g_i have the same number of vertices then the term $L_\beta(g_j; G)$ must result from a term in the expansion of (4) which does not involve δ functions. Then g_j is obtained from adding some edges to g_i. Therefore, g_i is a subgraph of g_j and g_j has more edges than g_i. The above properties are true for all α and β. For certain sets of α and β if $r_{\alpha\beta} = 0$ (see (3)), the element $t_{ij}^{\alpha\beta}$ is non-zero only if g_j contains fewer vertices than g_i. And if $q_{\alpha\beta} = s_{\alpha\beta} = 0$, $t_{ij}^{\alpha\beta}$ exists only if g_i is a subgraph of g_j.

From the above discussion, we can properly select a set of a finite number of graphs (for example, all connected graphs containing up to p vertices) and define the conversion matrix $T_{\alpha\beta}$ with elements $t_{ij}^{\alpha\beta}$ such that

$$L_\alpha = T_{\alpha\beta} \cdot L_\beta \tag{9}$$

where L_α and L_β are column vectors the elements of which are the lattice constants $L_\alpha(g_i; G)$ and $L_\beta(g_j; G)$ for the set of graphs considered. Among the eight lattice constant systems shown in table 2, there are 28 conversion matrices $T_{\alpha\beta}$ for each proper set of graphs considered. Not all of the matrices are independent.

From the procedure of expressing $L_\alpha(g_i; G)$ in terms of $L_\beta(g_j; G)$, it is easy to see that two matrices $T_{\alpha\beta}$ and $T_{\alpha'\beta'}$ are identical if

$$q_{\alpha\beta} = q_{\alpha'\beta'}, \qquad r_{\alpha\beta} = r_{\alpha'\beta'}, \qquad s_{\alpha\beta} = s_{\alpha'\beta'}, \tag{10a, b, c}$$

and

$$C_\beta(x, x) = C_{\beta'}(x, x), \qquad D_\beta(x, x) = D_{\beta'}(x, x), \tag{11a, b}$$

$$C_\beta(x, x')D_\beta(x, x') = C_{\beta'}(x, x')D_{\beta'}(x, x'). \tag{11c}$$

The above equations, however, cannot be simultaneously satisfied for any different pairs of $\alpha\beta$ and $\alpha'\beta'$. If $q_{\alpha\beta} = q_{\alpha'\beta'} = s_{\alpha\beta} = s_{\alpha'\beta'} = 0$, all the requirements described by (11) can be waived because no δ functions are involved. Then we have the identities $T_{1,2} = T_{3,4} = T_{5,8}$ and $T_{2,1} = T_{4,3} = T_{8,5}$. It is straightforward to see from (9) that $T_{\alpha\beta} = (T_{\beta\alpha})^{-1}$. We also note that for any γ, $T_{\alpha\beta} = T_{\alpha\gamma} \cdot T_{\gamma\beta} = T_{\alpha\gamma} \cdot (T_{\beta\gamma})^{-1}$. Therefore a knowledge of eight of the $T_{\alpha\beta}$, e.g. $T_{\alpha 1}$, gives any of the 28 T-matrices.

4. Reduction of lattice constants

Consider two graphs g_a and g_b. Each of them has a subgraph isomorphic to a complete graph g_c. (A graph is complete if all pairs of vertices are connected. The simplest complete graphs are single edge, triangle, etc.) If the two subgraphs are brought into coincidence, i.e. the two subgraphs are 'glued' together vertex by vertex and edge by edge, to form a graph g_r, then g_r is called a reducible graph. A graph which cannot be formed in this way is called irreducible. A reducible graph has the product property that

$$L_1(g_r; g) = L_1(g_a; G) \cdot L_1(g_b; G)/L_1(g_c; G), \tag{12}$$

provided G is a regular lattice. By regular lattice we mean that all vertices are equivalent and all edges are equivalent. The proof of (12) is simple and will not be given. We only note that if all edges of G are equivalent then all subgraphs of G which are isomorphic to a complete graph are equivalent.

In all lattice constant systems if G is a regular lattice, $L_\alpha(g_r; G)$ of a reducible graph g_r can be expressed in terms of lattice constants $L_\alpha(g_i; G)$ of irreducible graphs g_i. The numbers of vertices of g_i are equal to or less than the number of vertices of g_r. Examples of the reduction of lattice constants have been given by Domb (1960, 1974) for the weak lattice constant system L_3. We will show below why and how such a reduction can be done for an arbitrary lattice constant system L_α.

We first express $L_1(g_r; G)$ as a linear combination of $L_\alpha(g; G)$, i.e.

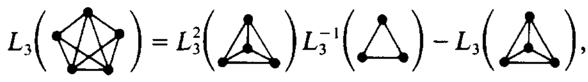
$$L_1(g_r; G) = L_\alpha(g_r; G) + \sum_{i \neq r} t_{ri}^{1\alpha} L_\alpha(g_i; G), \tag{13}$$

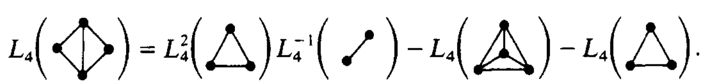
where we have used $t_{rr}^{1\alpha} = 1$, and separated the diagonal term from the summation. Since g_r is reducible, (13) can be rewritten as

$$L_\alpha(g_r; G) = \frac{L_1(g_a; G) \cdot L_1(g_b; G)}{L_1(g_c; G)} - \sum_{i \neq r} t_{ri}^{1\alpha} L_\alpha(g_i; G), \tag{14}$$

where we have made use of (12). Each graph g_a, g_b and g_c has a smaller number of vertices than g_r. The lattice constants $L_1(g_a; G)$, $L_1(g_b; G)$ and $L_1(g_c; G)$ can further be expressed in terms of $L_\alpha(g; G)$ with graphs g containing less vertices than g_r. Therefore, $L_\alpha(g_r; G)$ can be expressed in terms of lattice constants $L_\alpha(g_r'; G)$, where each graph g_r' either contains fewer vertices than g_r, or has the same number of vertices as g_r, but with more edges than g_r. If a graph g_r' is still reducible, we can repeat the same procedure and express $L_\alpha(g_r'; G)$ in terms of $L_\alpha(g_r''; G)$, etc. Eventually, $L_\alpha(g_r; G)$ is expressed in terms of lattice constants of irreducible graphs which have either the same number of vertices as g_r, or fewer vertices than g_r.

Two examples of the reduction of lattice constants are shown below:


(15)


(16)

The lattice constants $L_\alpha(g; G)$ are abbreviated as $L_\alpha(g)$ for simplicity.

5. Conclusions

We have considered eight different systems of extensive lattice constants. Some properties of these lattice constants are discussed. In particular we investigate a general method to express a lattice constant $L_\alpha(g_i; G)$ as a linear combination of $L_\beta(g_j; G)$. Such linear relations hold for any graph G. Properties of the coefficients $t_{ij}^{\alpha\beta}$ are also discussed. If the order (number of vertices) of g_i is low, the coefficients $t_{ij}^{\alpha\beta}$ can be obtained easily by the method described in § 3. For higher-order graphs g_i, the coefficients are difficult to determine manually. However, we can represent and identify graphs numerically (Chen and Lee 1981) and determine the coefficients by a computer. A straightforward application of the present method to relate L_1 in terms of L_3 has been carried out for graphs with up to nine edges. The results are too lengthy to be presented here, and will be published elsewhere.

For a regular lattice G, lattice constants $L_\alpha(g; G)$ of all reducible graphs (including all articulated graphs) can be expressed in terms of lattice constants of irreducible graphs. A general method to find the reduction of lattice constants has been described.

In this article lattice constants are defined only for unrooted graphs (i.e. all vertices are of the same species). If the graphs g are rooted (having different species of vertices), differented pairs of vertices may have different C_α (and C_α) functions. A large number of different lattice constant systems exist. But only a few of them are useful and need further studies.

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