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Dormant and Sprouts Generating Isospectral Tree Graphs. II. Theory

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Abstract

Existence and basic properties of the singlet and doublet dormants proposed in the preceding paper are rigorously proved and explained by using the topological index (Z) and Z-counting polynomial. Due to rapidly increasing complexity of multiplet dormants higher than triplet, mathematically incomplete but useful strategies for finding them are proposed and demonstrated.

1 Introduction

In the preceding paper [1] by demonstrating a variety of multiplet dormants it was convinced that the conventional endospectral graphs (ESG's) [2-4] are nothing else but "singlet dormants." There the topological index Z and Z-counting polynomial, or Q function, which have been proposed by the present author [5-7] are shown to work as useful key roles for finding these dormants without being bothered by solving eigen values of the characteristic polynomial. First, in this paper mathematical analysis will be performed for supporting the above techniques and results of the dormants with lower multiplicity. As the multiplicity increases the mathematical structure of this problem rapidly becomes entangled. However, thanks to our lucky situation many interesting results could be obtained by using several optimistic Conjectures and Expectations, which will be introduced and demonstrated as honestly as possible. Of course, systematic computerized survey is highly expected to amend the defect and sloppiness of the results of our back-of-envelop calculation.

2 Singlet dormant

First consider two graphs D and G. The host D has at least two vertices, while G only needs to have a root vertex. Then choose one vertex u from D, followed by giving a tentative name u to the root of G. We are going to attach G to D by identifying both u's to get graph C = GuD as illustrated in Figure 1. At this stage there is no restriction to choose u from D.

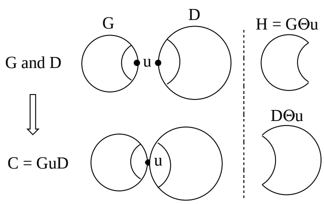


Figure 1. By identifying vertex u of G and D one gets Gud.

The Q function of GuD can be expressed by

$$Q_{\mathrm{GuD}} = Q_{\mathrm{H}}\, Q_{\mathrm{D}} + Q_{\mathrm{G}}\, Q_{\mathrm{D\Theta u}} - Q_{\mathrm{H}}\, Q_{\mathrm{D\Theta u}} \qquad (1)$$

according to the recursion formula obtained by the present author in 1973 [7] quite independently from Schwenk for characteristic polynomials [8].[1] Here DΘu is the graph obtained from D by deleting vertex u together with all the edges incident to u. Let GΘu be denoted simply by H. For

[1] In the case of characteristic polynomials ($P_{\mathrm{G}}(x)$) the corresponding expression is $Q_{\mathrm{GuD}} = Q_{\mathrm{H}}\, Q_{\mathrm{D}} + Q_{\mathrm{G}}\, Q_{\mathrm{D\Theta u}} - x\, Q_{\mathrm{H}}\, Q_{\mathrm{D\Theta u}}$. Notice the factor x multiplied to the last term of RHS of Eq. (1). However, $P_{\mathrm{G}}(x)$ will no longer be treated in this paper.

later discussion instead of using Q_f let us simply use *f* in italic to represent its *Q* function. Then Eq. (1) can be changed into a slimmer expression as

$$GuD = H\,D + (G - H)\,(D\Theta u) \qquad (2)$$

If G is simply an edge, G=1+x and H=1, giving

$$GuD = D + x\,(D\Theta u). \qquad (3)$$

By putting x=1 into Eq. (3) one gets

$$Z(\mathrm{GuD}) = Z(\mathrm{D}) + Z(\mathrm{D\Theta u}), \qquad (4)$$

which is found to be very useful in checking the isospectrality of graphs, where G is and edge.

Now try to choose another vertex v from D, and rename u of G as v. Then the *Q* of GvD obtained by identifying both v's of G and D can be expressed by

$$GvD = H\,D + (G - H)\,(D\Theta v) \qquad (5)$$

By comparing Eqs. (2) and (5) we get important Theorem 1, which also governs the conventional ESG discussion.

[Theorem 1]   (singlet dormant)

If a pair of graphs GuD and GvD are isospectral, then $D\Theta u = D\Theta v$. vice versa.

Namely Theorem 1 is the necessary and sufficient condition for the existence of the singlet dormant in the realm of tree graphs. Let us call such subgraphs of D like DΘu and DΘv as "pre-dormants" in the discussion of dormants. We have checked that the *Q*'s of the pre-dormants of all the 64 examples of endospectral trees in the paper by Knop et al. [9] fulfill Theorem 1. Here one may add the following Corollary.

[Corollary 1] (singlet dormant)

If a pair of graphs GuD and GvD are isospectral, then $Z(D\Theta u) = Z(D\Theta v)$. Namely, the Z's of their pre-dormants are the same. However, the reverse is not necessarily true, but highly probable.

Let us take **1**~**3** as an example for realizing Theorem 1. Graph **1** (=D) in Fig. 2 has been known as the smallest endospectral tree to generate a pair of IS trees, **2** and **3** [3,8].

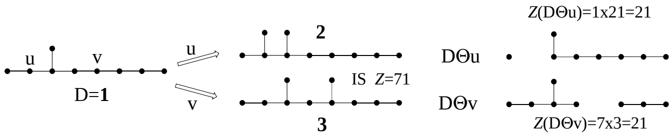


Figure 2. Smallest singlet dormant D generates a pair of IS trees.

By applying Eq. (3) to **2** and **3** one gets

$$C_2 = D + x\,(D\Theta u) \text{ and } C_3 = D + x\,(D\Theta v), \qquad (6)$$

where the Q of D has already been obtained to be $D=1+8x+20x^2+17x^3+4x^4$ [6]. $D\Theta u$ and $D\Theta v$ can be calculated by using the easily obtainable [2,3,5-7] Q's of small graphs to be $D\Theta u=1+6x+10x^2+4x^3$ and $D\Theta v=(1+4x+2x^2)(1+2x)$ $=1+6x+10x^2+4x^3$. Then we get $C_2= C_3=1+9x+26x^2+27x^3+8x^4$. By putting x=1 in these polynomials, we get

$$Z_1=Z(D)=50, \quad Z(D\Theta u)=21, \quad \text{and} \quad Z(D\Theta v)=7\times 3=21.$$

By using Eq. 4 we have $Z_2=Z_3=71$.

We can understand why **1** is the smallest singlet dormant, or ESG, in the tree graphs by drawing the whole map of the Z values of all the candidates of pre-dormants, $Z(D\Theta u)$, of **1** as in Fig. 3, where only a pair of vertices are found to have the same $Z(D\Theta u)$ values as encircled.

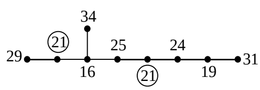


Figure 3: The Z values of the subgraph DΘu for all the vertices of **1**. The encircled vertices become the sprouts of the singlet dormant.

All other tree graphs below N≤9 are found to have no duplicate Z(DΘu) value among their symmetrically independent vertices. A rigorous mathematical proof can be reached by switching the above discussion from the Z index to the Q function.

Next we will show an interesting property of a singlet dormant, which already has ben known for non-tree ESG's but without sophisticated discussion [10,11]. Try to attach graphs G and E to dormant D with two sprouts u and v to generate a pair of GuDvE and EuDvG as in Fig. 4.

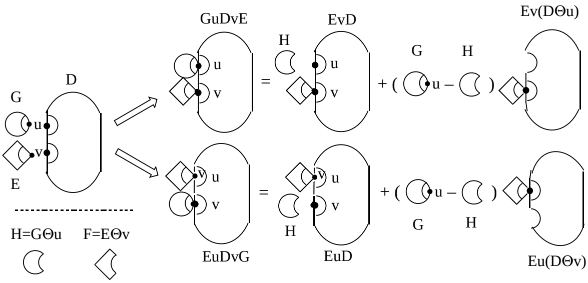


Figure 4. A pair of graphs GuDvE and EuDvG are constructed from G, E, and D. The two pairs, GuD and GvD, and EuD and EvD, are isospectral within each other.

By using Eq. (1) the Q functions of both the graphs can be expressed as (See Fig. 4)

$$G\mathrm{u}D\mathrm{v}E = H(E\mathrm{v}D) + (G - H)\{E\mathrm{v}(D\Theta u)\} \tag{7}$$

and

$$E\mathrm{u}D\mathrm{v}G = H(E\mathrm{u}D) + (G - H)\{E\mathrm{u}(D\Theta v)\}. \tag{8}$$

Since the vertices u and v are the sprouts of dormant D,

$$E\mathrm{v}D = E\mathrm{u}D. \tag{9}$$

Although we know the equality of the following pair of Q functions as

$$D\Theta u = D\Theta v, \tag{10}$$

the equality of the Q's of the pair of graphs, Ev(DΘu) and Eu(DΘv) (as shown in the right-most part of Fig. 4) is not yet proved at this stage. By using Eq. (1) these *Q*'s can be expressed, respectively, as

$$E\mathrm{v}(D\Theta u) = F(D\Theta u) + (E - F)(D\Theta uv) \tag{11}$$

and

$$E\mathrm{u}(D\Theta v) = F(D\Theta v) + (E - F)(D\Theta uv), \tag{12}$$

where $D\Theta uv$ is the *Q* of the graph obtained from D by deleting u and v together with all the edges incident to u and v.

Then by using Eq. (10) we get

$$E\mathrm{v}(D\Theta u) = E\mathrm{u}(D\Theta v), \tag{13}$$

trace back through Eqs. (7) and (8), and finally reach the desired result as

$$G\mathrm{u}D\mathrm{v}E = E\mathrm{u}D\mathrm{v}G, \tag{14}$$

which ensures

[Theorem 2] (*XDY*=*YDX* of singlet dormant)

Singlet dormant D (tree) with a pair of sprouts, u and v, generates an IS pair of XuDvY and YuDvX,

by using a pair of rooted graphs, X and Y.[2]

3 Doublet dormant

Consider a doublet dormant such as **4** in Fig. 5 [12], which has two pairs of sprouts (u_1, u_2) and (v_1, v_2), and generates an IS tree pairs (Gu_1u_2D and Gv_1v_2D) as **5** and **6** by adding a pair of edges to those sprouts (See Figure 6a).

[2] X and Y can be chosen from non-tree graphs, but we are not going into detailed discussion here.

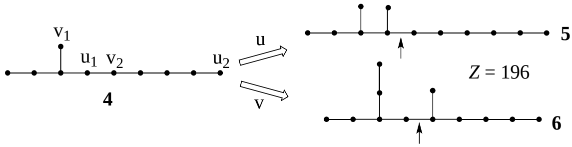


Figure 5. Example of a doublet dormant **4** generating IS graphs, **5** and **6**.

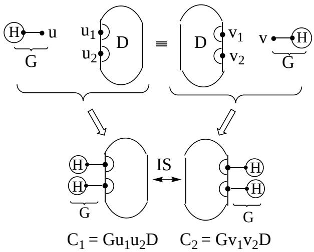


Figure 6a. Doublet dormant

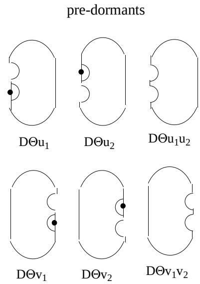


Figure 6b. Various pre-dormants

After repeated calculation using Eq. (1) the following pair of expressions for the *Q* functions of jointed graphs C_1 = Gu_1u_2D and C_2 = Gv_1v_2D can be obtained as Eqs. (15) and (16). The relevant pre-dormants are shown in Fig. 6b. Especially when G is an edge, the corresponding *Z* values can be obtained as Eqs. (17) and (18).

$$C_1 = H^2 D + H (G - H) \{(D\Theta u_1) + (D\Theta u_2)\} + (G - H)^2 (D\Theta u_1u_2) \quad (15)$$

$$C_2 = H^2 D + H (G - H) \{(D\Theta v_1) + (D\Theta v_2)\} + (G - H)^2 (D\Theta v_1v_2) \quad (16)$$

$$Z (\mathrm{Gu_1u_2D}) = Z (\mathrm{D}) + \{Z (\mathrm{D\Theta u_1}) + Z (\mathrm{D\Theta u_2})\} + Z (\mathrm{D\Theta u_1u_2}) \quad (17)$$

$$Z (\mathrm{Gv_1v_2D}) = Z (\mathrm{D}) + \{Z (\mathrm{D\Theta v_1}) + Z (\mathrm{D\Theta v_2})\} + Z (\mathrm{D\Theta v_1v_2}) \quad (18)$$

From Eqs. (15) and (16) the following theorem for doublet dormants can be derived.

[Theorem 3] (doublet dormant)

For graph D with two pairs of vertices (u_1, u_2) and (v_1, v_2), if (i) $D\Theta u_1u_2 = D\Theta v_1v_2$ and (ii) $\Sigma(D\Theta u) = \Sigma(D\Theta v)$, then Gu_1u_2D and Gv_1v_2D become an IS pair, both of which are generated from the doublet dormant D.

[Expectation 1] (doublet dormant)

For graph D with two pairs of vertices (u_1, u_2) and (v_1, v_2), if (i) $Z(D\Theta u_1u_2)=Z(D\Theta v_1v_2)$ and (ii) $\Sigma Z(D\Theta u)=\Sigma Z(D\Theta v)$, then it is highly possible that Gu_1u_2D and Gv_1v_2D become an IS pair, both of which are generated from the doublet dormant D.

Theorem 3 is indeed a sufficient condition for $C_1=C_2$. However, it is very difficult to find such IS pair graphs that do not have the property of (i) and (ii) simultaneously. On the other hand, Expectation 1 is not actually a corollary but just an expectation by the present author. Namely, there is no mathematical rigorousness in it. However, as will be shown in this paper it has a strong strategic role for finding dormants very effectively.

Instead of pursuing mathematical rigorousness let us make sure how Theorem 3 and Expectation 1 hold true in concrete examples. Consider graph **4** which generates an IS pair **5** and **6**. Further, when G is an edge, the Q functions necessary for applying Eqs. (15) and (16) are given in Figure 7.

Now by assembling (*1)~(*3) in Figure 7 we get

$$C_1 = C_2 = (*1) + x\,(*2) + x^2\,(*3) = 1 + 11\,x + 43\,x^2 + 73\,x^3 + 53\,x^4 + 14\,x^5 + x^6 \tag{19}$$

as already given in Eq. (6) of the preceding paper. The Z indices can be obtained by putting x=1 into the above formulas as

$$Z\,(C_1) = Z\,(C_2) = 81 + 90 + 25 = 196, \tag{20}$$

which is the same as Eq. (7) of the preceding paper.

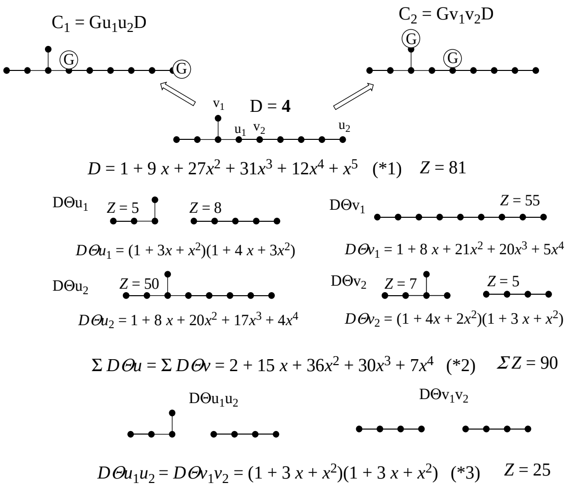


Figure 7. *Q* functions for supporting Eqs. (15) and (16) for the case with **4~6**. G is chosen as an edge.

Then try to find other doublet dormants. We could not find any doublet dormant among the tree graphs with N=5 and 6, but many among those with N=7 as already shown in Figure 6 of the preceding paper. Rapid increase with N from here might be expected.

4 Triplet dormant

Next consider a triplet dormant D as in Figure 8 which has two pairs of three sprouts (u_1, u_2, u_3) and (v_1, v_2, v_3), and generates an IS tree pair ($Gu_1u_2u_3D$ and $Gv_1v_2v_3D$) by adding an edge to each of their sprouts.

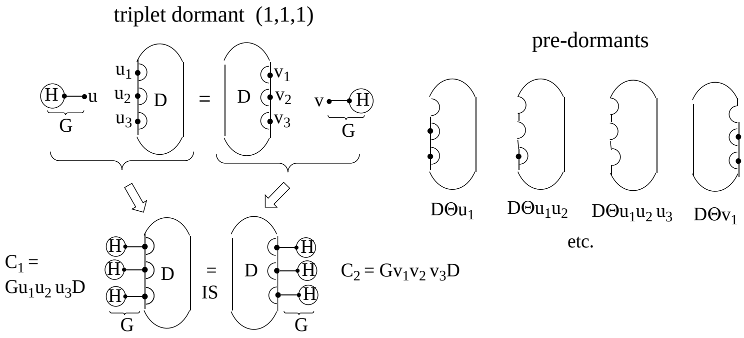


Figure 8. Triplet dormant and its pre-dormants.

By performing a similar manipulation as in the case of the doublet dormant in Figure 6 we get the *Q* function and *Z* index of jointed graph $Gu_1u_2u_3D$ as follows:

$$Gu_1u_2u_3D = H^3 D + H^2 (G - H) \{(D\Theta u_1) + (D\Theta u_2) + (D\Theta u_3)\}$$
$$+ H (G - H)^2\{(D\Theta u_1u_2) + (D\Theta u_1u_3) + (D\Theta u_2u_3)\}$$
$$+ (G - H)^3 (D\Theta u_1u_2u_3) \qquad (21)$$

$$Z(Gu_1u_2u_3D) = Z(D) + \{Z(D\Theta u_1) + Z(D\Theta u_2) + Z(D\Theta u_3)\}$$
$$+ \{Z(D\Theta u_1u_2) + Z(D\Theta u_1u_3) + Z(D\Theta u_2u_3)\}+ Z(D\Theta u_1u_2u_3) \qquad (22)$$

Here G is also supposed to be an edge in Eq. (22). The pre-dormants in these expressions are also shown in Figure 8. It is interesting to observe that for the case with G=1+x and H=1 Eq. (21) is turned into the form

$$Gu_1u_2u_3D = D + x\,\Sigma(D\Theta u_1) + x^2\,\Sigma(D\Theta u_1u_2) + x^3\,(D\Theta u_1u_2u_3). \qquad (23)$$

Similarly for the *Z* index in the case where G is an edge we get

$$Z(Gu_1u_2u_3D) = Z(D) + \Sigma Z(D\Theta u_1) + \Sigma Z(D\Theta u_1u_2) + Z(D\Theta u_1u_2u_3). \qquad (24)$$

By following the above manipulations we get Theorem 4.

[Theorem 4]   (triplet dormant (1,1,1))

For graph D with two pairs of vertices (u_1, u_2, u_3) and (v_1, v_2, v_3), if (i) $D\Theta u_1u_2u_3=D\Theta v_1v_2v_3$,

(ii) $\Sigma(D\Theta u_1u_2)=\Sigma(D\Theta v_1v_2)$, (iii) $\Sigma(D\Theta u_1)=\Sigma(D\Theta v_1)$, then $Gu_1u_2u_3D$ and $Gv_1v_2v_3D$ become an IS pair, both of which are generated from the triplet dormant D.

In this case also this is a sufficient condition for $C_1=C_2$. However, it is very difficult to find such IS pair graphs that do not have all the properties (i)~(iii) at all.

As in the case with doublet dormants we would like to propose Expectation 2.

[Expectation 2]   (triplet dormant (1,1,1))

For graph D with two pairs of vertices (u_1, u_2, u_3) and (v_1, v_2, v_3), if (i) $Z(D\Theta u_1u_2u_3)=Z(D\Theta v_1v_2v_3)$,

(ii) $\Sigma Z(D\Theta u_1u_2)=\Sigma Z(D\Theta v_1v_2)$, and (iii) $\Sigma Z(D\Theta u_1)= \Sigma Z(D\Theta v_1)$, then it is highly possible that

$Gu_1u_2u_3D$ and $Gv_1v_2v_3D$ become an IS pair, both of which are generated from the triplet dormant D.

Anyway a concrete example for supporting Theorem 4 and Expectation 2 is given in Figure 9 for the case with triplet dormant **7** (N=6) and the IS pair **8** and **9** which are derived from it. They were already introduced in Fig. 4 of the preceding paper.

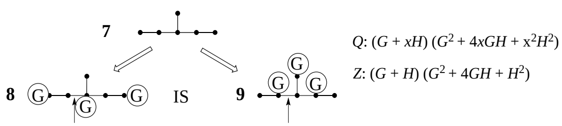


Figure 9. Triplet dormant generating mirror-symmetric IS pair graphs.

It is to be noted that Theorem 4 and Expectation 2 do not directly apply to the triplet dormant **10** and the derived IS pair **11** and **12**, because Eqs. (21) and (22) were derived for the dormant whose sprouts (u_1, u_2, u_3) and (v_1, v_2, v_3) grow, respectively, from all different vertices. On the other hand, in both of **11** and **12** two sprouts grow from the same vertex. Namely, there are found two different types in the family of triplet dormants, i.e., (1,1,1) and (1,2) types.

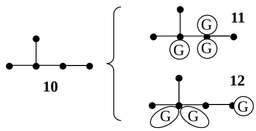


Figure 10. Triplet dormant in which three sprouts grow from two vertices.

As the former graphs have already been discussed in Figure 8 and Theorem 4, we are going to discuss the latter. See Figure 11, where (1,2)-type triplet dormant D and the resultant graph C=$Gu_1G'u_2D$ are demonstrated with the relevant pre-dormants. This C is obtained by identifying the single and double sprouts, u_1 and u_2, with the roots of the attaching graphs G and G', respectively.

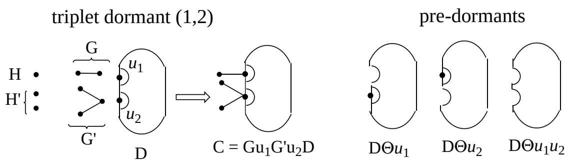


Figure 11. (1,2)-Type triplet dormant and the relevant pre-dormants.

The *Q* function of C is obtained to be

$$C = Gu_1G'u_2D = H\,H'\,D + (G - H)\,H'\,(D\Theta u_1) + (G' - H')\,H\,(D\Theta u_2)$$
$$+\ (G - H)\,(G' - H')\,(D\Theta u_1u_2). \qquad (25)$$

The expression for the corresponding *Z* index can easily be obtained from Eq. (25) in parallel with the case of Eqs. (21) and (22) as

$$Z(\mathrm{C}) = Z(\mathrm{D}) + Z(\mathrm{D}\Theta \mathrm{u}_1) + 2Z(\mathrm{D}\Theta \mathrm{u}_2) + 2Z(\mathrm{D}\Theta \mathrm{u}_1\mathrm{u}_2). \qquad (26)$$

Note that this expression seems to be essentially the same as Eq. (24) if those sprouts attached to the same vertex are not allowed to be included in the summation.

By applying Eq. (25) to **11** and **12** one gets

$$C\,(\mathbf{11}) = H\,H'\,(1+4x+2x^2) + (G-H)\,H'\,(1+x) + (G'-H')\,H\,(1+2x) + (G-H)\,(G'-H') \qquad (27)$$

and

$$C\,(\mathbf{12}) = H\,H'\,(1+4x+2x^2) + (G-H)\,H'\,(1+3x) + (G'-H')\,H\,(1+x) + (G-H)\,(G'-H'). \qquad (28)$$

Note that in both the graphs, the vertices u_1 and u_2 are chosen, respectively, for single and double sprouts. Then in the special case with **11** and **12**, as G=1+x, H=1, G'=1+2x, and H'=1, we get the same results as

$$C\,(\mathbf{11}) = (1+4x+2x^2) + x(1+x) + 2x(1+2x) + 2x^2 = 1 + 7x + 9x^2, \qquad (29)$$ and

$$C\,(\mathbf{12}) = (1+4x+2x^2) + x(1+3x) + 2x(1+x) + 2x^2 = 1 + 7x + 9x^2. \qquad (30)$$

5 Multiplet dormants in general

We have hitherto seen that multiplet dormants not only encompass the concept of the endospectral graph and vertices but also have various interesting features of IS tree graphs. Although the necessary conditions for their existence seem to get more complicated rapidly with their multiplicity, we found that we are in a lucky situation in search of finding highly multiplet dormants as suggested in Eqs. (23) and (24).

This situation will be shown in the case with another IS pair of **13** and **14** derived from the same graph **10**, but quadruplet dormant in this case. Initially they were found from our list of the four IS pair tree graphs with N=9 (See **16** and **17** in Fig. 4 of the preceding paper) [1], but this fact was confirmed by the following check.

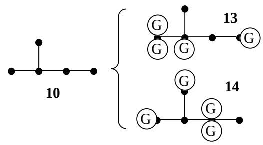


Figure 12. Quadruplet dormant in which four sprouts grow from three vertices.

First assume the existence of IS pair(s) with *N*=9 derived from dormant **10** by growing four edges from its various sprouts whose distribution is allowed to be either (1,1,1,1), (1,1,2), or (2,2). Then they should be in the list of Figure 13 prepared according to the conditions prescribed above. In this case twenty-nine candidates were listed up among which **13** and **14** are included.

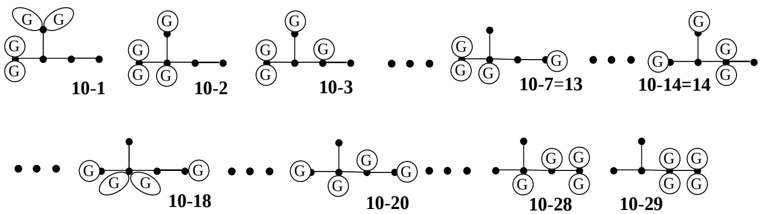
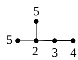


Figure 13. *N*=9 tree graphs derived from the smallest dormant **10** by adding four edges, G's.

We can calculate their *Z*-indices, *Z*(I)'s, of all these graphs, which scatter in the range of 21~48. Then try to calculate the sum of the *Z*'s of pre-dormants, $\Sigma Z(D\Theta u_1)$, which appeared in Eqs. (24) and (26). For this purpose the following diagram  is useful which gives the *Z* values of the pre-dormants for the component vertices. Then each of the 29 graphs in Figure 13 is given a set of two numbers, *Z*(C) and $\Sigma Z(D\Theta u_1)$. As the candidates for the IS pairs only the following two pairs were found to have the same set, namely, **10-7** (or **13**) and **10-14** (or **14**) with (36, 16) and **10-18** and **10-28** with (31, 13).

Finally we have to calculate the *Q* functions of these four graphs. Although details are not given here, the obtained results are as follows,

$$C_{13} = C_{14} = 1 + 8x + 17x^2 + 10x^3,$$

$$C_{10\text{-}18} = 1 + 8x + 15x^2 + 7x^3,$$

and
$$C_{10\text{-}28} = 1 + 8x + 16x^2 + 6x^3. \quad (31)$$

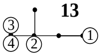
Then we can conclude that **13** and **14** are the only IS pair which are derived from the quadruplet dormant **10**. On the other hand, **10-18** and **10-28** are not IS but IZ (iso-*Z*) pair graphs. The conclusion already declared for the results shown in Figure 5 has been obtained after this line of analysis, including the check against the possibility of growing more than three sprouts from one vertex.

As shown above we could select the candidates for the IS pairs without tedious check of the *Q* functions of a large number of candidates but only with simple manipulation of their *Z* indices and $\Sigma Z(\mathrm{D}\Theta u_1)$ values.

Furthermore, unexpected and useful results were obtained by calculating the values of $\Sigma Z(\mathrm{D}\Theta u_1u_2)$ and $\Sigma Z(\mathrm{D}\Theta u_1u_2u_3)$ of **13** and **14** as in Figure 14.

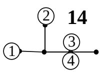
Namely, it was found that the *Z* indices of both **13** and **14** can be correctly calculated by using Eq. (24) as 36=7+16+11+2. Similarly for both **10-18** and **10-28** we could get the correct results as 31=7+13+9+2. The difference between these two pairs seems to come from the terms $\Sigma Z(\mathrm{D}\Theta u_1)$ and $\Sigma Z(\mathrm{D}\Theta u_1u_2)$.

13



(u_1u_2)	(12)	(13)	(14)	(23)	(24)		$(u_1u_2u_3)$	(123)	(124)	
$\Sigma Z(\mathrm{D}\Theta u_1u_2) =$	1	+ 3	+ 3	+ 2	+ 2	= 11	$\Sigma Z(\mathrm{D}\Theta u_1u_2u_3) =$	1	+ 1	= 2

14



(u_1u_2)	(12)	(13)	(14)	(23)	(24)		$(u_1u_2u_3)$	(123)	(124)	
$\Sigma Z(\mathrm{D}\Theta u_1u_2) =$	3	+ 2	+ 2	+ 2	+ 2	= 11	$\Sigma Z(\mathrm{D}\Theta u_1u_2u_3) =$	1	+ 1	= 2

Figure 14. Calculation of $\Sigma Z(\mathrm{D}\Theta u_1u_2)$ and $\Sigma Z(\mathrm{D}\Theta u_1u_2u_3)$ of **13** and **14**.

The Q functions of **13** and **14** were also correctly obtained by using Eq. (23) as

$$C_{13} = C_{14} = (1+4x+2x^2)+x(4+10x+2x^2)+x^2(5+6x)+ x^3(2)=1+8x+17x^2+10x^3, \qquad (32)$$

while the Q functions of the pair **10-18**,**28** were found to be different from each other as expected.

Although we cannot get any mathematical proof for this lucky situation, let us optimistically assume the following expectation and conjecture.

[Expectation 3] (multiplet dormant)

For a pair of IZ graphs, $Gu_1u_2\ldots u_sD$ and $Gv_1v_2\ldots v_sD$, derived from graph D by attaching s edges one by one to two pairs of vertices ($u_1, u_2,\cdots, u_s$) and ($v_1, v_2,\cdots, v_s$), if (i) $\Sigma Z(D\Theta u_1u_2\ldots u_s) = \Sigma Z(D\Theta v_1v_2\ldots v_s)$ and (ii) $\Sigma Z(D\Theta u_1)=\Sigma Z(D\Theta v_1)$, then it is highly possible that these graphs are IS derived from multi(s)plet dormant D.

[Conjecture 1] (multiplet dormant)

The Q function of the graph $I=Gu_1u_2\cdots u_sD$ obtained from dormant D composed of d vertices by attaching s edges one by one to the sprouts $u_1, u_2,\cdots, u_s$ which are distributed among t ($\leq d,s$) vertices is obtained to be

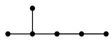
$$Gu_1u_2\cdots u_sD = D + x\,\Sigma(D\Theta u_1) + x^2\,\Sigma(D\Theta u_1u_2) + \cdots\ x^t\,\Sigma(D\Theta u_1u_2\ldots u_t). \qquad (33)$$

Eq. (33) can be deemed as a formal extension of Eq. (23). Note that in the summation below $\Sigma(D\Theta u_1u_2)$ in RHS of Eq. (33) only one sprout u should be selected from one vertex.

Conjecture 1 seems to assert that one needs to make sure of one to one correspondence between each term in RHS of Eq. (33) to check if a pair of graphs are IS. Curiously enough it was found that the value of the first summation is enough for checking isospectrality among the above

29 graphs.

We will add one more example of our lucky situation for finding multiplet dormant and the IS pair graphs derived from it. Amazingly the tree graph



15

was found to work not only as a triplet dormant, but also quadruplet, sextuplet, octuplet, and nonuplet dormants to generate a variety of IS graphs.

Here let us demonstrate how the two nonuplet items were discovered by using Expectation 3. First assume the existence of IS tree pair(s) with N=15 derived from **15** by growing nine edges from its various sprouts whose distribution is either (1,1,1,2,2,2) or (1,2,2,2,2) type. Here no other type like (2,2,2,3) is assumed to be allowed. Quite similarly to the case with Fig. 13 the aimed pair(s) should be in the list of Fig. 15 prepared according to the prescribed conditions.

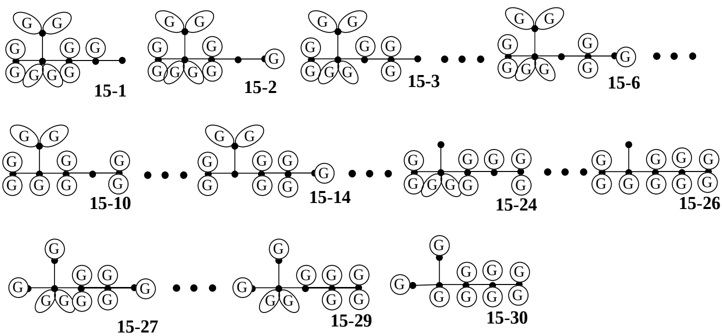
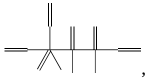


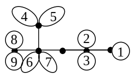
Figure 15. N=15 tree graphs derived from dormant **15** by attaching nine G's.

Now assume again that G is an edge. Then we calculated the Z-indices of these 30 graphs, which scattered in the wide range of 323~471. Among them we could find four pairs with the same Z's, namely, **15-3**,**24** (333), **15-6**,**26** (360), **15-10**,**27** (396), and **15-14**,**29** (408). Note that in the above trees only **15-27~30** graphs were found to have non-zero p(G,6), as suggested from the following diagram,

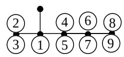


while **15-1~26** cannot. Then we can conclude that the last two pairs cannot be IS.

Now try to check graphs **15-6**,**26**. As Z(D)=Z(**15**)=11, the next step is the calculation of the values of ΣZ(DΘu_1) and of the terms that follow in the RHS of Eq. (33). Although each term for these two graphs is different as seen in Figure 16, their sums were found to be the same as 53. The sums of the Q functions (ΣZ$D\Theta u_1$)) of their pre-dormants were also calculated to be equal.



15-6



15-26

u_1	$D\Theta u_1$	$Z(D\Theta u_1)$	u_1	$D\Theta u_1$	$Z(D\Theta u_1)$
1	$1+4x+2x^2$	7	1	$1+2x$	3
2,3	$1+3x$	4	2,3	$1+4x+3x^2$	8
4,5	$1+4x+3x^2$	8	4,5	$(1+x)(1+2x)=1+3x+2x^2$	6
6,7	$1+2x$	3	6,7	$1+3x$	4
8,9	$1+4x+3x^2$	8	8,9	$1+4x+2x^2$	7
Σ	$9+30x+14x^2$	53	Σ	$9+30x+14x^2$	53

Figure 16. Calculation of $\Sigma D\Theta u_1$ and $\Sigma Z(D\Theta u_1)$ of **15-6**,**26**

Although details are not given here, we could obtain ΣZ(DΘu_1u_2), ΣZ(DΘ$u_1u_2u_3$), ΣZ(DΘ$u_1u_2u_3u_4$), and ΣZ(DΘ$u_1u_2u_3u_4u_5$), respectively, to be 104, 112, 64, and 16 for both the graphs. Now we have 11+53+104+112+64+16=360. Further, by calculating all the corresponding Q functions our Conjecture 2 was supported in this case.

Quite similarly we could show that another pair **15-3**,**24** was found to be nonuplet IS. In this way we could also enjoy our Expectation 3.

6 Concluding remark

We have exposed rather clumsy methodology for finding multiplet dormants for generating IS tree graphs by the manipulation of the Z index without recourse to any computer search on a large scale. However, once candidates for an IS pair are found, its fair judgment is quite easily obtained. Further, as already mentioned, the finding of multiplet dormants encompasses the conventional discussions concerning the endospectral graphs and vertices.

However, the present author is eagerly waiting for more systematic and mathematical survey of this problem. There are so many interesting and important problems which are relevant to the mathematical structure and properties of the multiplet dormants in many fields, such as conjugated polyenes, aromatic hydrocarbons, and QSAR studies in chemistry, several inverse problems in physics, fundamental problems of spectra of graphs in mathematics, etc. Especially in chemistry, this line of analysis should be extended to weighted and/or non-tree graphs leading to the basic discussion on the origin of aromaticity.

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