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Some Indices in the Random Spiro Chains

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ABSTRACT

The Gutman index, Schultz index, multiplicative degree-Kirchhoff index, additive degree-Kirchhoff index are four well-studied topological indices, which are useful tools in QSPR and QSAR investigations. Spiro compounds are an important class of cycloalkanes in organic chemistry. In this paper, we determine the expected values of these indices in the random spiro chains, and the extremal values among all spiro chains with n hexagons.

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1. INTRODUCTION

Throughout this paper, all graphs we considered are finite, undirected, and simple. Let $G = (V, E)$ be a connected graph with $n = |V|$ vertices and $m = |E|$ edges. For a vertex $v \in V(G)$, the degree of u, denote by $d_G(u)$ (short for $d(u)$), is the number of vertices which are adjacent to u. The distance $d(u, v)$, is the length of a shortest path between u and v. The resistance distance $r(u, v)$, is the effective resistance between u and v. Denote $d(u|G) = \sum_{v\in V(G)} d(u, v)$ and $r(u|G) = \sum_{v\in V(G)} r(u, v)$. Other notations and terminologies not defined here will conform to those in [1].

Topological indices are the graph invariants used in theoretical chemistry to encode molecules for the design of chemical compounds with given physicochemical properties or given pharmacological and biological activities [2].

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Among all the topological indices, the most well-known is the Wiener index [4], which is defined as $W(G) = \sum_{\{u,v\}\subseteq V(G)} d_G(u,v)$. As a weighted version of the Wiener index, Gutman index and Schultz index [5] was proposed as

$$Gut(G) = \sum_{\{u,v\}\subseteq V(G)}(d_G(u)d_G(v))d_G(u,v),$$
$$S(G) = \sum_{\{u,v\}\subseteq V(G)}(d_G(u) + d_G(v))d_G(u,v).$$

Similarly, if the distance is replaced by resistance distance in the expression for the Gutman index and Schultz index, respectively, then one arrives the multiplicative degree-Kirchhoff index and additive degree-Kirchhoff index.

The multiplicative degree-Kirchhoff index was proposed by Chen et al. in [6], and defined as

$$Kf^*(G) = \sum_{\{u,v\}\subseteq V(G)}(d_G(u)d_G(v))r_G(u,v),$$

where $r_G(u,v)$ is the resistance distance between vertex u and v in G. Gutman et al. defined in [7] the additive degree-Kirchhoff index as

$$Kf^+(G) = \sum_{\{u,v\}\subseteq V(G)}(d_G(u) + d_G(v))r_G(u,v).$$

The research on the topological indices of some special chemical chains and their application in chemistry has become a hot issue in chemical graph theory. In [8], Huang et al. obtained exact formulas for the expected values of the Kirchhoff indices of the random polyphenyl and spiro chains. Recently, Geng et al. [9] got the Kirchhoff indices and the number of spanning trees of möbius phenylenes chain and cylinder phenylenes chain. Došlić et al. [3] introduced a new bond-additive invariant of a connected graph, named the Mostar index, as a measure of peripherality in graphs. They gave a cut method for computing the Mostar index of benzenoid systems and posed an open problem: Find extremal benzenoid chains, catacondensed benzenoids and general benzenoid graphs with respect to the Mostar index. Later, Xiao et al. [10, 11] partially solve the problem. They determined the first three maximal and minimal values of the Mostar index among all hexagonal chains with h hexagons, and characterize the corresponding extremal graphs by some transformations on hexagonal chains. Other results see [12−18] and the references cited therein.

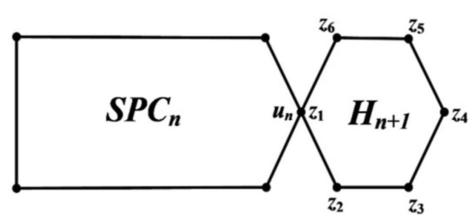

Figure 1. A spiro chain SPC_{n+1} with $n + 1$ hexagons.

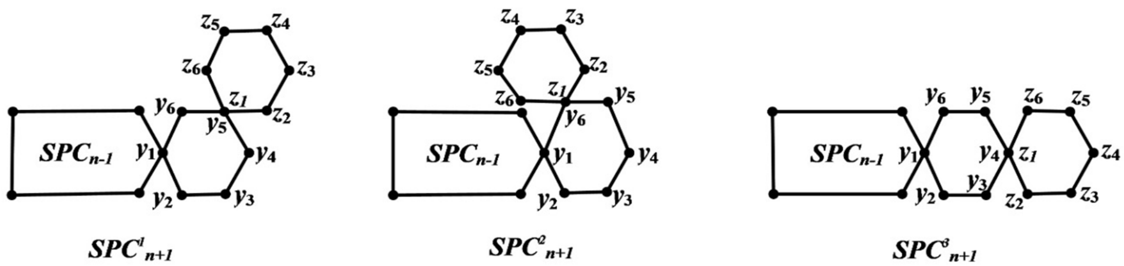

Figure 2. The three types of local arrangements in spiro chains.

A spiro chain SPC_{n+1} with $n+1$ hexagons can be regarded as a spiro chain SPC_n with n hexagons to which a new terminal hexagon H_{n+1} has been adjoined, see Figure [1].

For $n \geq 3$, the terminal hexagon H_{n+1} can be attached in three ways, which results in the local arrangements, we describe as SPC^1_{n+1}, SPC^2_{n+1} and SPC^3_{n+1}, respectively, see Figure [2].

A random spiro chain SPC_n with n hexagons is a spiro chain obtained by stepwise addition of terminal hexagons. At each step $t(=3,4,\ldots,n)$, a random selection is made from one of the three possible constructions:

i. $SPC_{t-1} \rightarrow SPC^1_t$ with probability p_1;
ii. $SPC_{t-1} \rightarrow SPC^2_t$ with probability p_2;
iii. $SPC_{t-1} \rightarrow SPC^3_t$ with probability $1-p_1-p_2$, where p_1, p_2 are constants, irrelative to the step parameter t.

We denote by $SPC_n(1,0)$, $SPC_n(0,1)$, $SPC_n(0,0)$, the spiro meta-chain M_n, the spiro orth-chain O_n, the spiro para-chain P_n, respectively.

Motivated by [17], we explore the properties of these indices of spiro chain. In this paper, we determine the expected values of Gutman index $E(Gut(SPC_n(p_1, p_2)))$, Schultz index $E(S(SPC_n(p_1, p_2))$, multiplicative degree-Kirchhoff index $E(Kf^*(SPC_n(p_1, p_2)))$, additive degree-Kirchhoff index $E(Kf^+(SPC_n(p_1, p_2)))$ in the random spiro chains and the extremal values of these indices among all spiro chains with n hexagons. We also give the average values of these indices among all spiro chains with n hexagons.

2. THE GUTMAN INDEX OF SPC_n

The Gutman index of a random spiro chain $SPC_n(p_1, p_2)$ (or SPC_n for short) is random variable. In the following, we calculate the expected value of $Gut(SPC_n)$. Denote SPC_{n+1} the graph obtained by attaching SPC_n a new terminal hexagon H_{n+1} which is spanned by vertices z_1, z_2, z_3, z_4, z_5, z_6 and z_1 is u_n, see Figure 1.

It is obvious that, for all $v \in SPC_n$,

$d(v, z_1) = d(v, u_n)$; $d(v, z_2) = d(v, u_n) + 1$; $d(v, z_3) = d(v, u_n) + 2$;
$d(v, z_4) = d(v, u_n) + 3$; $d(v, z_5) = d(v, u_n) + 2$; $d(v, z_6) = d(v, u_n) + 1$;
$\sum_{v\in V(SPC_n)} d_{SPC_{n+1}}(v) = 12n + 2$.

We also have that

$\sum_{i=1}^{6} d(z_i)d(z_i, z_1) = 18$; $\sum_{i=1}^{6} d(z_i)d(z_i, z_2) = 20$; $\sum_{i=1}^{6} d(z_i)d(z_i, z_3) = 22$;
$\sum_{i=1}^{6} d(z_i)d(z_i, z_4) = 24$; $\sum_{i=1}^{6} d(z_i)d(z_i, z_5) = 22$; $\sum_{i=1}^{6} d(z_i)d(z_i, z_6) = 20$.

Denote by $E(Gut(SPC_n(p_1, p_2)))$ the expected value of Gutman index of the random spiro chain $SPC_n(p_1, p_2)$.

Theorem 2.1. For $n \geq 1$, we have $E(Gut(SPC_n(p_1, p_2))) = (72 - 24p_1 - 48p_2)n^3 + (72p_1 + 144p_2)n^2 + (36 - 48p_1 - 96p_2)n$.

Proof. We proof it in the Appendix A.1. ■

If $(p_1, p_2) = (1, 0)$, then $SPC_n \cong M_n$; If $(p_1, p_2) = (0, 1)$, then $SPC_n \cong O_n$; If $(p_1, p_2) = (0, 0)$, then $SPC_n \cong P_n$. From Theorem 2.1, we have

Corollary 2.2. The Gutman index of the para-chain P_n, the meta-chain M_n and the ortho-chain O_n are

$$Gut(P_n) = 72n^3 + 36n;$$
$$Gut(M_n) = 48n^3 + 72n^2 - 12n;$$
$$Gut(O_n) = 24n^3 + 144n^2 - 60n.$$

Corollary 2.3. Among all spiro chains with $n(n \geq 3)$ hexagons, the graphs with the minimum and the maximum Gutman index are the ortho-chain O_n and the para-chain P_n, respectively.

Proof. Let SPC_n be a spiro chain with n hexagons. By Theorem 2.1, one knows that $f_1(p_1, p_2) = E(Gut(SPC_n))=(-24n^3 + 72n^2 - 48n)\, p_1 + (-48n^3 + 144n^2 - 96n)\, p_2 + 72n^3 + 36n$. As $n \geq 3$, we have that $\frac{\partial f_1}{\partial p_1} = -24n^3 + 72n^2 - 48n < 0$; $\frac{\partial f_1}{\partial p_2} = -48n^3 + 144n^2 - 96n < 0$.

Note that $0 \leq p_1 \leq 1$, $0 \leq p_2 \leq 1$, $0 \leq p_1 + p_2 \leq 1$, then $f_1(p_1, p_2) \leq 72n^3 + 36n$, with equality if and only if $p_1 = p_2 = 0$, it means that SPC_n is para-chain P_n.

On the other hand,

$$f_1(p_1, p_2) = (-24n^3 + 72n^2 - 48n)(p_1 + p_2) + (-24n^3 + 72n^2 - 48n)p_2 + 72n^3 + 36n$$

$$\geq (-24n^3 + 72n^2 - 48n) \times 1 + (-24n^3 + 72n^2 - 48n)p_2 + 72n^3 + 36n$$
$$= (-24n^3 + 72n^2 - 48n)p_2 + 48n^3 + 72n^2 - 12n$$
$$\geq (-24n^3 + 72n^2 - 48n) \times 1 + 48n^3 + 72n^2 - 12n$$
$$\geq 24n^3 + 144n^2 - 60n,$$

with equality if and only if $p_1 + p_2 = 1$ and $p_2 = 1$, i.e. $p_1 = 0$ and $p_2 = 1$, it means that SPC_n is ortho-chain O_n. This completes the proof. ■

3. THE SCHULTZ INDEX OF SPC_n

The Schultz index of a random spiro chain SPC_n is random variable. In the following, we calculate the expected value of $S(SPC_n)$. Denote by $E(S(SPC_n(p_1, p_2)))$ the expected value of Schultz index of the random spiro chain $SPC_n(p_1, p_2)$.

Theorem 3.1. For $n \geq 1$, we have $E(S(SPC_n(p_1, p_2))) = (60 - 20p_1 - 40p_2)n^3 + (60p_1 + 120p_2 + 18)n^2 + (30 - 40p_1 - 80p_2)n$.

Proof. We proof it in the Appendix A.2. ■

If $(p_1, p_2) = (1,0)$, then $SPC_n \cong M_n$; If $(p_1, p_2) = (0,1)$, then $SPC_n \cong O_n$; If $(p_1, p_2) = (0,0)$, then $SPC_n \cong P_n$. From Theorem 3.1, we have the following corollary:

Corollary 3.2. The Schultz index of the para-chain P_n, the meta-chain M_n and the ortho-chain O_n are

$$S(P_n) = 60n^3 + 18n^2 + 30n;$$
$$S(M_n) = 40n^3 + 78n^2 - 10n;$$
$$S(O_n) = 20n^3 + 138n^2 - 40n.$$

Corollary 3.3. Among all spiro chains with $n(n \geq 3)$ hexagons, the graphs with the minimum and the maximum Schultz index are the ortho-chain O_n and the para-chain P_n, respectively.

Proof. Let SPC_n be a spiro chain with n hexagons. By Theorem 3.1, one knows that $f_2(p_1, p_2) = E(S(SPC_n)) = (-20n^3 + 60n^2 - 40n)\, p_1 + (-40n^3 + 120n^2 - 80n)\, p_2 + 60n^3 + 18n^2 + 30n$. As $n \geq 3$, we have that $\frac{\partial f_2}{\partial p_1} = -20n^3 + 60n^2 - 40n < 0$; $\frac{\partial f_2}{\partial p_2} = -40n^3 + 120n^2 - 80n < 0$.

Note that $0 \leq p_1 \leq 1$, $0 \leq p_2 \leq 1$, $0 \leq p_1 + p_2 \leq 1$, then $f_2(p_1, p_2) \leq 60n^3 + 18n^2 + 30n$, with equality if and only if $p_1 = p_2 = 0$, it means that SPC_n is para-chain P_n.

On the other hand, we have

$$f_2(p_1, p_2) = (-20n^3 + 60n^2 - 40n)(p_1 + p_2) + (-20n^3 + 60n^2 - 40n)p_2 + 60n^3 + 18n^2 + 30n$$
$$\geq (-20n^3 + 60n^2 - 40n) \times 1 + (-20n^3 + 60n^2 - 40n)p_2 + 60n^3 + 18n^2 + 30n$$
$$= (-20n^3 + 60n^2 - 40n)p_2 + 40n^3 + 78n^2 - 10n$$
$$\geq (-20n^3 + 60n^2 - 40n) \times 1 + 40n^3 + 78n^2 - 10n$$
$$\geq 20n^3 + 138n^2 - 40n,$$

with equality if and only if $p_1 + p_2 = 1$ and $p_2 = 1$, i.e. $p_1 = 0$ and $p_2 = 1$, it means that SPC_n is ortho-chain O_n. This completes the proof. ■

4. THE MULTIPLICATIVE DEGREE–KIRCHHOFF INDEX OF SPC_n

The multiplicative degree-Kirchhoff index of a random spiro chain SPC_n is random variable. In the following, we calculate the expected value of $Kf^*(SPC_n)$.

It is obvious that, for all $v \in SPC_n$,

$r(v, z_1) = r(v, u_n; r(v, z_2) = r(v, u_n) + \frac{5}{6}; r(v, z_3) = r(v, u_n) + \frac{4}{3}; r(v, z_4) = r(v, u_n) + \frac{3}{2}; r(v, z_5) = r(v, u_n) + \frac{4}{3}; r(v, z_6) = r(v, u_n) + \frac{5}{6}; \sum_{v \in V(SPC_n)} d_{SPC_{n+1}}(v) = 12n + 2.$

We also have that

$$\sum_{i=1}^{6} d(z_i) r(z_i, z_1) = \frac{35}{3}; \sum_{i=1}^{6} d(z_i) r(z_i, z_2) = \frac{40}{3}; \sum_{i=1}^{6} d(z_i) r(z_i, z_3) = \frac{43}{3};$$
$$\sum_{i=1}^{6} d(z_i) r(z_i, z_4) = \frac{44}{3}; \sum_{i=1}^{6} d(z_i) r(z_i, z_5) = \frac{43}{3}; \sum_{i=1}^{6} d(z_i) r(z_i, z_6) = \frac{40}{3}.$$

Denote by $E(Kf^*(SPC_n(p_1, p_2)))$ the expected value of multiplicative degree-Kirchhoff index of the random spiro chain $SPC_n(p_1, p_2)$.

Theorem 4.1. For $n \geq 1$, we have $E(Kf^*(SPC_n(p_1, p_2))) = (36 - 4p_1 - 16p_2)n^3 + (32 + 12p_1 + 48p_2)n^2 + (2 - 8p_1 - 32p_2)n$.

Proof. We proof it in the Appendix A.3. ■

If $(p_1, p_2) = (1, 0)$, then $SPC_n \cong M_n$; If $(p_1, p_2) = (0, 1)$, then $SPC_n \cong O_n$; If $(p_1, p_2) = (0, 0)$, then $SPC_n \cong P_n$. From Theorem 4.1, we have

Corollary 4.2. The multiplicative degree-Kirchhoff index of the para-chain P_n, the meta-chain M_n and the ortho-chain O_n are

$$Kf^*(P_n) = 36n^3 + 32n^2 + 2n;$$
$$Kf^*(M_n) = 32n^3 + 44n^2 - 6n;$$
$$Kf^*(O_n) = 30n^3 + 80n^2 - 30n.$$

Corollary 4.3. Among all spiro chains with $n(n \geq 3)$ hexagons, the graphs with the minimum and the maximum multiplicative degree-Kirchhoff index are the ortho-chain O_n and the para-chain P_n, respectively.

Proof. Let SPC_n be a spiro chain with n hexagons. By Theorem 4.1, one knows that $f_3(p_1, p_2) = E(Kf^*(SPC_n)) = (-4n^3 + 12n^2 - 8n)\, p_1 + (-16n^3 + 48n^2 - 32n)\, p_2 + 36n^3 + 32n^2 + 2n$. As $n \geq 3$, we have that $\frac{\partial f_3}{\partial p_1} = -4n^3 + 12n^2 - 8n < 0$; $\frac{\partial f_3}{\partial p_2} = -16n^3 + 48n^2 - 32n < 0$.

Note that $0 \leq p_1 \leq 1$, $0 \leq p_2 \leq 1$, $0 \leq p_1 + p_2 \leq 1$, then $f_3(p_1, p_2) \leq 36n^3 + 32n^2 + 2n$, with equality if and only if $p_1 = p_2 = 0$, it means that SPC_n is para-chain P_n.

On the other hand, we have

$$\begin{aligned} f_3(p_1, p_2) &= (-4n^3 + 12n^2 - 8n)(p_1 + p_2) + (-12n^3 + 36n^2 - 24n)p_2 + 36n^3 \\ &\quad + 32n^2 + 2n \\ &\geq (-4n^3 + 12n^2 - 8n) \times 1 + (-12n^3 + 36n^2 - 24n)p_2 + 36n^3 + \\ &\quad 32n^2 + 2n \\ &= (-12n^3 + 36n^2 - 24n)p_2 + 32n^3 + 44n^2 - 6n \\ &\geq (-12n^3 + 36n^2 - 24n) \times 1 + 32n^3 + 44n^2 - 6n \\ &\geq 30n^3 + 80n^2 - 30n, \end{aligned}$$

with equality if and only if $p_1 + p_2 = 1$ and $p_2 = 1$, i.e. $p_1 = 0$ and $p_2 = 1$, it means that SPC_n is ortho-chain O_n. This completes the proof. ■

5. THE ADDITIVE DEGREE−KIRCHHOFF INDEX OF SPC_n

The additive degree-Kirchhoff index of a random spiro chain SPC_n is random variable. In the following, we calculate the expected value of $Kf^+(SPC_n)$. Denote by $E(Kf^+(SPC_n(p_1, p_2)))$ the expected value of additive degree-Kirchhoff index of the random spiro chain $SPC_n(p_1, p_2)$.

Theorem 5.1. For $n \geq 1$, we have $E(Kf^+(SPC_n(p_1, p_2))) = (30 - \frac{10}{3}p_1 - \frac{40}{3}p_2)n^3 + (115 + 10p_1 + 40p_2)n^2 + (\frac{5}{3} - \frac{20}{3}p_1 - \frac{80}{3}p_2)n.$

Proof. We proof it in the Appendix A.4. ■

If $(p_1, p_2) = (1, 0)$, then $SPC_n \cong M_n$; If $(p_1, p_2) = (0, 1)$, then $SPC_n \cong O_n$; If $(p_1, p_2) = (0, 0)$, then $SPC_n \cong P_n$. From Theorem 5.1, we have

Corollary 5.2. The additive degree-Kirchhoff index of the para-chain P_n, the meta-chain M_n and the ortho-chain O_n are

$$Kf^+(P_n) = 30n^3 + 115n^2 + \frac{5}{3}n;$$
$$Kf^+(M_n) = \frac{80}{3}n^3 + 125n^2 - 15n;$$
$$Kf^+(O_n) = \frac{50}{3}n^3 + 115n^2 - 25n.$$

Corollary 5.3. Among all spiro chains with n $(n \geq 3)$ hexagons, the graphs with the minimum and the maximum additive degree-Kirchhoff index are the ortho-chain O_n and the para-chain P_n, respectively.

Proof. Let SPC_n be a spiro chain with n hexagons. By Theorem 5.1, one knows that $f_4(p_1, p_2) = E(Kf^+(SPC_n))$=$(-\frac{10}{3}n^3 + 10n^2 - \frac{20}{3}n)\, p_1$ +$(-\frac{40}{3}n^3 + 40n^2 - \frac{80}{3}n)\, p_2$ + $30n^3 + 115n^2 + \frac{5}{3}n$. As $n \geq 3$, we have that $\frac{\partial f_4}{\partial p_1} = -\frac{10}{3}n^3 + 10n^2 - \frac{20}{3}n < 0$; $\frac{\partial f_4}{\partial p_2} = -\frac{40}{3}n^3 + 40n^2 - \frac{80}{3}n < 0$.

Note that $0 \leq p_1 \leq 1$, $0 \leq p_2 \leq 1$, $0 \leq p_1 + p_2 \leq 1$, then $f_4(p_1, p_2) \leq 30n^3 + 115n^2 + \frac{5}{3}n$, with equality if and only if $p_1 = p_2 = 0$, it means that SPC_n is para-chain P_n.

On the other hand, we have

$$\begin{aligned} f_4(p_1, p_2) &= \left(-\frac{10}{3}n^3 + 10n^2 - \frac{20}{3}n\right)(p_1 + p_2) + (-10n^3 + 30n^2 - 20n)p_2 + 30n^3 \\ &\quad + 115n^2 + \frac{5}{3}n \\ &\geq \left(-\frac{10}{3}n^3 + 10n^2 - \frac{20}{3}n\right) \times 1 + (-10n^3 + 30n^2 - 20n)p_2 + 30n^3 + \\ &\quad 115n^2 + \frac{5}{3}n \\ &= (-10n^3 + 30n^2 - 20n)p_2 + \frac{80}{3}n^3 + 125n^2 - 5n \\ &\geq (-10n^3 + 30n^2 - 20n) \times 1 + \frac{80}{3}n^3 + 125n^2 - 5n \\ &\geq \frac{50}{3}n^3 + 155n^2 - 25n, \end{aligned}$$

with equality if and only if $p_1 + p_2 = 1$ and $p_2 = 1$, i.e. $p_1 = 0$ and $p_2 = 1$, it means that SPC_n is ortho-chain O_n. This completes the proof. ■

6. AVERAGE VALUES OF THESE INDICES

Denote by $\mathcal{H}_n$ the set of all spiro chains with n hexagons. The average value of these indices among $\mathcal{H}_n$ can be characterized as

$$Gut_{avr}(\mathcal{H}_n) = \frac{1}{|\mathcal{H}_n|}\sum_{G\in\mathcal{H}_n} Gut(G); \quad S_{avr}(\mathcal{H}_n) = \frac{1}{|\mathcal{H}_n|}\sum_{G\in\mathcal{H}_n} S(G);$$
$$Kf^*_{avr}(\mathcal{H}_n) = \frac{1}{|\mathcal{H}_n|}\sum_{G\in\mathcal{H}_n} Kf^*(G); Kf^+_{avr}(\mathcal{H}_n) = \frac{1}{|\mathcal{H}_n|}\sum_{G\in\mathcal{H}_n} Kf^+(G).$$

If $(p_1, p_2) = (\frac{1}{3}, \frac{1}{3})$, then we can obtain the average value. By Theorems 2.1, 3.1, 4.1, 5.1, we have the following result.

Theorem 6.1. The average values of these indices among $\mathcal{H}_n$ are

$$Gut_{avr}(\mathcal{H}_n) = 48n^3 + 72n^2 - 12n; \; S_{avr}(\mathcal{H}_n) = 40n^3 + 78n^2 - 10n;$$
$$Kf^*_{avr}(\mathcal{H}_n) = \frac{88}{3}n^3 + 52n^2 - \frac{34}{3}n; Kf^+_{avr}(\mathcal{H}_n) = \frac{40}{3}n^3 + \frac{395}{3}n^2 - \frac{95}{3}n.$$

We can find that $Gut_{avr}(\mathcal{H}_n) = Gut(M_n)$ and $S_{avr}(\mathcal{H}_n) = S(M_n)$. It means that we can use the spiro chain M_n to characterize the average value of $\mathcal{H}_n$ with respect to Gutman index and Schultz index.

A Appendix

A.1 Proof of Theorem 2.1

Proof. Let $Gut(SPC_{n+1}) = A_1 + B_1 + C_1$, where $A_1 = \sum_{\{u,v\}\subseteq SPC_n} d(u)d(v)d(u,v)$; $B_1 = \sum_{v\in SPC_n\setminus\{u_n\}}\sum_{z_i\in H_{n+1}\setminus\{z_1\}} d(v)d(z_i)d(v,z_i)$; $C_1 = \sum_{\{z_i,z_j\}\subseteq H_{n+1}} d(z_i)d(z_j)d(z_i,z_j)$.

$$\begin{aligned}A_1 &= \sum_{\{u,v\}\subseteq SPC_n\setminus\{v_n\}} d(u)d(v)d(u,v) + \sum_{v\in SPC_n\setminus\{v_n\}} d_{SPC_{n+1}}(u_n)d(v)d(u_n,v),\\ &= \sum_{\{u,v\}\subseteq SPC_n\setminus\{v_n\}} d(u)d(v)d(u,v) + \sum_{v\in SPC_n\setminus\{v_n\}}\big(d_{SPC_n}(u_n) + 2\big)d(v)d(u_n,v),\\ &= Gut(SPC_n) + 2\sum_{v\in SPC_n} d(v)d(u_n,v).\end{aligned}$$

$$\begin{aligned}B_1 &= \sum_{v\in SPC_n}\sum_{z_i\in H_{n+1}} d(v)d(z_i)d(v,z_i)\\ &\quad -4\sum_{v\in SPC_n} d(v)d(v,u_n) - 4\sum_{v\in H_{n+1}} d(v)d(v,z_1),\\ &= \sum_{v\in SPC_n} d(v)[4d(v,u_n) + 4(d(v,u_n)+1) + 4(d(v,u_n)+2) + 2(d(v,u_n) +\\ &\quad 3)] - 4\sum_{v\in SPC_n} d(v)d(v,u_n) - 4\times 18,\\ &= 10\sum_{v\in SPC_n} d(v)d(v,u_n) + 18(12n-2).\end{aligned}$$

$$C_1 = \frac{1}{2}\sum_{i=1}^{6} d(z_i)\left(\sum_{j=1}^{6} d(z_j)d(z_j,z_i)\right) = \frac{1}{2}(4\times 18 + 4\times 20 + 4\times 22 + 2\times 24) = 144.$$

Thus, $Gut(SPC_{n+1}) = Gut(SPC_n) + 12\sum_{v\in SPC_n} d(v)d(v,u_n) + 216n + 108$. As $SPC_n(p_1,p_2)$ is a random spiro chain, $\sum_{v\in SPC_n} d(v)d(v,u_n)$ is a random variable. Denote $U_n^1 \coloneqq E\big(\sum_{v\in SPC_n} d(v)d(v,u_n)\big)$. Then $E(Gut(SPC_{n+1})) = E(Gut(SPC_n)) + 12U_n^1 + 216n + 108$.

In the following, we calculate U_n^1 by considering three possible cases.

Case 1. $SPC_n \to SPC_{n+1}^1$.

$u_n(z_1)$ coincides with y_5 or y_3 (see Figure 2), thus $\sum_{v\in SPC_n} d(v)d(v,u_n)$ is given by $\sum_{v\in SPC_n} d(v)d(v,y_5)$ with probability p_1.

Case 2. $SPC_n \to SPC_{n+1}^2$.

$u_n(z_1)$ coincides with y_6 or y_2 (see Figure 2), thus $\sum_{v\in SPC_n} d(v)d(v,u_n)$ is given by $\sum_{v\in SPC_n} d(v)d(v,y_6)$ with probability p_2.

Case 3. $SPC_n \to SPC_{n+1}^3$.

$u_n(z_1)$ coincides with y_4 (see Figure 2), thus $\sum_{v\in SPC_n} d(v)d(v,u_n)$ is given by $\sum_{v\in SPC_n} d(v)d(v,y_4)$ with probability $p_3 = 1 - p_1 - p_2$.

From Case 1, Case 2 and Case 3, we have that

$$\begin{aligned}
U_n^1 &= p_1 \sum_{v\in SPC_n} d(v)d(v,y_5) + p_2 \sum_{v\in SPC_n} d(v)d(v,y_6) \\
&\quad +(1 - p_1 - p_2) \sum_{v\in SPC_n} d(v)d(v,y_4), \\
&= p_1\Big[\sum_{v\in SPC_{n-1}} d(v)d(v,u_{n-1}) + 2\sum_{v\in SPC_{n-1}\setminus\{v_{n-1}\}} d(v) + 22\Big] \\
&\quad + p_2\Big[\sum_{v\in SPC_{n-1}} d(v)d(v,u_{n-1}) + \sum_{v\in SPC_{n-1}\setminus\{v_{n-1}\}} d(v) + 20\Big] \\
&\quad +(1 - p_1 - p_2)\Big[\sum_{v\in SPC_{n-1}} d(v)d(v,u_{n-1}) + 3\sum_{v\in SPC_{n-1}\setminus\{v_{n-1}\}} d(v) + 24\Big] \\
&= p_1(U_{n-1}^1 + 24n - 6) + p_2(U_{n-1}^1 + 12n + 6) + (1 - p_1 - p_2)(U_{n-1}^1 + 36n - 18) \\
&= U_{n-1}^1 + (36 - 12p_1 - 24p_2)n + (12p_1 + 24p_2 - 18).
\end{aligned}$$

And the initial value is $U_1^1 = \sum_{v\in SPC_1} d(v)d(v,u_1) = 18$. Thus,

$$U_n^1 = (18 - 6p_1 - 12p_2)n^2 + (6p_1 + 12p_2)n. \tag{1}$$

So,

$$\begin{aligned}
E(Gut(SPC_{n+1})) &= E(Gut(SPC_n)) + 12U_n^1 + 216n + 108, \\
&= E\big(Gut(SPC_n)\big) + 72(3 - p_1 - 2p_2)n^2 + 72(3 + p_1 + 2p_2)n + 108.
\end{aligned}$$

Since the initial value is $E\big(Gut(SPC_1)\big) = 2 \times 2 \times 6 \times \frac{1}{2} \times (1 \times 2 + 2 \times 2 + 3) = 108$,

$$E\big(Gut(SPC_n)\big) = (72 - 24p_1 - 48p_2)n^3 + (72p_1 + 144p_2)n^2 + (36 - 48p_1 - 96p_2)n$$

This completes the proof. ∎

A.2 Proof of Theorem 3.1

Proof. Let $S(SPC_{n+1}) = A_2 + B_2 + C_2$, where $A_2 = \sum_{\{u,v\}\subseteq SPC_n}(d(u) + d(v))d(u,v)$; $B_2 = \sum_{v\in SPC_n\setminus\{u_n\}} \sum_{z_i\in H_{n+1}\setminus\{z_1\}}(d(v) + d(z_i))d(v,z_i)$;
$C_2 = \sum_{\{z_i,z_j\}\subseteq H_{n+1}}(d(z_i) + d(z_j))d(z_i,z_j)$.

$A_2 = \sum_{\{u,v\}\subseteq SPC_n\setminus\{v_n\}}(d(u) + d(v))d(u,v) + \sum_{v\in SPC_n\setminus\{v_n\}}(d_{SPC_{n+1}}(u_n) + d(v))d(u_n,v),$
$= \sum_{\{u,v\}\subseteq SPC_n\setminus\{v_n\}}(d(u) + d(v))d(u,v) + \sum_{v\in SPC_n\setminus\{v_n\}}\left(d_{SPC_n}(u_n) + 2 + d(v)\right)d(u_n,v),$
$= S(SPC_n) + 2\sum_{v\in SPC_n} d(u_n,v)$
$= S(SPC_n) + 2d(u_n|SPC_n).$

$B_2 = \sum_{v\in SPC_n}\sum_{z_i\in H_{n+1}}(d(v) + d(z_i))d(v,z_i) - \sum_{v\in SPC_n}(d(v) + 4)d(v,u_n) - \sum_{v\in H_{n+1}}(d(v) + 4)d(v,z_1),$
$= \sum_{v\in SPC_n} d(v)[d(v,u_n) + 2(d(v,u_n) + 1) + 2(d(v,u_n) + 2) + 2(d(v,u_n) + 3)] + \sum_{v\in SPC_n}[4d(v,u_n) + 4(d(v,u_n) + 1) + 4(d(v,u_n) + 2) + 2(d(v,u_n) + 3)] - \sum_{v\in SPC_n} d(v)d(v,u_n) - 4\sum_{v\in SPC_n} d(v,u_n) - 54,$
$= 5\sum_{v\in SPC_n} d(v)d(v,u_n) + 10d(u_n|SPC_n) + 198n - 18.$

$C_2 = \sum_{i=1}^{6} d(z_i)\left(\sum_{j=1}^{6} d(z_j,z_i)\right) = 9 \times (4 + 2 \times 5) = 126.$

Thus, $S(SPC_{n+1}) = S(SPC_n) + 5\sum_{v\in SPC_n} d(v)d(v,u_n) + 12d(u_n|SPC_n) + 198n + 108$. As $SPC_n(p_1,p_2)$ is a random spiro chain, $d(u_n|SPC_n)$ is a random variable. Denote $U_n^2 := E(d(u_n|SPC_n))$. Then $E(S(SPC_{n+1})) = E(S(SPC_n)) + 5U_n^1 + 12U_n^2 + 198n + 108$.

In the following, we calculate U_n^2 by considering three possible cases.

Case 1. $SPC_n \to SPC_{n+1}^1$.
$u_n(z_1)$ coincides with y_5 or y_3 (see Figure 2), thus $d(u_n|SPC_n)$ is given by $d(y_5|SPC_n)$ with probability p_1.

Case 2. $SPC_n \to SPC_{n+1}^2$.
$u_n(z_1)$ coincides with y_6 or y_2 (see Figure 2), thus $d(u_n|SPC_n)$ is given by $d(y_6|SPC_n)$ with probability p_2.

Case 3. $SPC_n \to SPC_{n+1}^3$.
$u_n(z_1)$ coincides with y_4 (see Figure 2), thus $d(u_n|SPC_n)$ is given by $d(y_4|SPC_n)$ with probability $p_3 = 1 - p_1 - p_2$.

From Case 1, Case 2 and Case 3, we have that
$U_n^2 = p_1 d(y_5|SPC_n) + p_2 d(y_6|SPC_n) + (1 - p_1 - p_2)d(y_4|SPC_n),$
$= p_1[d(u_{n-1}|SPC_{n-1}) + 2(5n - 5) + 9] + p_2[d(u_{n-1}|SPC_{n-1}) + (5n - 5) + 9] + (1 - p_1 - p_2)[d(u_{n-1}|SPC_{n-1}) + 3(5n - 5) + 9],$

$= p_1(U_{n-1}^2 + 10n - 1) + p_2(U_{n-1}^2 + 5n + 4) + (1 - p_1 - p_2)(U_{n-1}^2 + 15n - 6),$
$= U_{n-1}^2 + (15 - 5p_1 - 10p_2)n + (5p_1 + 10p_2 - 6).$

And the initial value is $U_1^2 = d(u_1|SPC_1) = 9$. Thus, $U_n^2 = \frac{1}{2}(15 - 5p_1 - 10p_2)n^2 + \frac{1}{2}(5p_1 + 10p_2 + 3)n$. From equation 1, $U_n^1 = (18 - 6p_1 - 12p_2)n^2 + (6p_1 + 12p_2)n$. We have,

$$E(S(SPC_{n+1})) = E(S(SPC_n)) + 5U_n^1 + 12U_n^2 + 198n + 108,$$
$$= E(S(SPC_n)) + 60(3 - p_1 - 2p_2)n^2 + 12(18 + 5p_1 + 10p_2)n + 108.$$

Since the initial value is $E(S(SPC_1)) = 9 \times 6 \times 2 = 108$, so

$$E(S(SPC_n)) = (60 - 20p_1 - 40p_2)n^3 + (18 + 60p_1 + 120p_2)n^2 + (30 - 40p_1 - 80p_2)n$$

This completes the proof. ∎

A.3 Proof of Theorem 4.1

Proof. Let $Kf^*(SPC_{n+1}) = A_3 + B_3 + C_3$, where $A_3 = \sum_{\{u,v\}\subseteq SPC_n} d(u)d(v)r(u,v)$; $B_3 = \sum_{v\in SPC_n\backslash\{u_n\}} \sum_{z_i\in H_{n+1}\backslash\{z_1\}} d(v)d(z_i)r(v,z_i)$; $C_3 = \sum_{\{z_i,z_j\}\subseteq H_{n+1}} d(z_i)d(z_j)r(z_i,z_j)$.

$$A_3 = \sum_{\{u,v\}\subseteq SPC_n\backslash\{v_n\}} d(u)d(v)r(u,v) + \sum_{v\in SPC_n\backslash\{v_n\}} d_{SPC_{n+1}}(u_n)d(v)r(u_n,v),$$
$$= \sum_{\{u,v\}\subseteq SPC_n\backslash\{v_n\}} d(u)d(v)r(u,v) + \sum_{v\in SPC_n\backslash\{v_n\}} \left(d_{SPC_n}(u_n) + 2\right)d(v)r(u_n,v),$$
$$= Kf^*(SPC_n) + 2\sum_{v\in SPC_n} d(v)r(u_n,v).$$

$$B_3 = \sum_{v\in SPC_n}\sum_{z_i\in H_{n+1}} d(v)d(z_i)r(v,z_i) - 4\sum_{v\in SPC_n} d(v)r(v,u_n) - 4\sum_{v\in H_{n+1}} d(v)r(v,z_1),$$
$$= \sum_{v\in SPC_n} d(v)\left[4r(v,u_n) + 4\left(r(v,u_n) + \frac{5}{6}\right) + 4\left(r(v,u_n) + \frac{4}{3}\right) + 2\left(r(v,u_n) + \frac{3}{2}\right)\right] - 4\sum_{v\in SPC_n} d(v)r(v,u_n) - 4 \times \frac{35}{3},$$
$$= 10\sum_{v\in SPC_n} d(v)r(v,u_n) + \frac{35}{3}(12n - 2).$$

$$C_3 = \frac{1}{2}\sum_{i=1}^{6} d(z_i)\left(\sum_{j=1}^{6} d(z_j)r(z_j,z_i)\right) = \frac{1}{2}\left(4 \times \frac{35}{3} + 4 \times \frac{40}{3} + 4 \times \frac{43}{3} + 2 \times \frac{44}{3}\right) = \frac{280}{3}.$$

Thus, $Kf^*(SPC_{n+1}) = Kf^*(SPC_n) + 12\sum_{v\in SPC_n} d(v)r(v,u_n) + 140n + 70$. As $SPC_n(p_1,p_2)$ is a random spiro chain, $\sum_{v\in SPC_n} d(v)r(v,u_n)$ is a random variable. Denote $U_n^3 := E\left(\sum_{v\in SPC_n} d(v)r(v,u_n)\right)$. Then $\mathrm{E}(Kf^*(SPC_{n+1})) = E(Kf^*(SPC_n)) + 12U_n^3 + 140n + 70.$

In the following, we calculate U_n^3 by considering three possible cases.

Case 1. $SPC_n \to SPC_{n+1}^1$.

$u_n(z_1)$ coincides with y_5 or y_3 (see Figure 2), thus $\sum_{v\in SPC_n} d(v)r(v,u_n)$ is given by $\sum_{v\in SPC_n} d(v)r(v,y_5)$ with probability p_1.

Case 2. $SPC_n \to SPC_{n+1}^2$.

$u_n(z_1)$ coincides with y_6 or y_2 (see Figure 2), thus $\sum_{v\in SPC_n} d(v)r(v,u_n)$ is given by $\sum_{v\in SPC_n} d(v)r(v,y_6)$ with probability p_2.

Case 3. $SPC_n \to SPC_{n+1}^3$.

$u_n(z_1)$ coincides with y_4 (see Figure 2), thus $\sum_{v\in SPC_n} d(v)r(v,u_n)$ is given by $\sum_{v\in SPC_n} d(v)r(v,y_4)$ with probability $p_3 = 1 - p_1 - p_2$.

From Case 1, Case 2 and Case 3, we have that

$$\begin{aligned}
U_n^3 &= p_1 \textstyle\sum_{v\in SPC_n} d(v)r(v,y_5) + p_2 \sum_{v\in SPC_n} d(v)r(v,y_6) \\
&\quad +(1 - p_1 - p_2)\textstyle\sum_{v\in SPC_n} d(v)r(v,y_4), \\
&= p_1\left[\textstyle\sum_{v\in SPC_{n-1}} d(v)r(v,u_{n-1}) + 2\sum_{v\in SPC_{n-1}\setminus\{v_{n-1}\}} d(v) + \frac{34}{3}\right] \\
&\quad +p_2\left[\textstyle\sum_{v\in SPC_{n-1}} d(v)r(v,u_{n-1}) + \sum_{v\in SPC_{n-1}\setminus\{v_{n-1}\}} d(v) + \frac{40}{3}\right] \\
&\quad +(1 - p_1 - p_2)\left[\textstyle\sum_{v\in SPC_{n-1}} d(v)r(v,u_{n-1}) + 3\sum_{v\in SPC_{n-1}\setminus\{v_{n-1}\}} d(v) + \frac{44}{3}\right], \\
&= p_1(U_{n-1}^3 + 16n - \tfrac{13}{3}) + p_2(U_{n-1}^3 + 10n + \tfrac{5}{3}) + (1 - p_1 - p_2)(U_{n-1}^3 + 18n - \tfrac{19}{3}), \\
&= U_{n-1}^3 + (18 - 2p_1 - 8p_2)n + (2p_1 + 8p_2 - \tfrac{19}{3}).
\end{aligned}$$

And the initial value is $U_1^3 = \sum_{v\in SPC_1} d(v)r(v,u_1) = \frac{35}{3}$. Thus,

$$U_n^3 = (9 - p_1 - 4p_2)n^2 + (\tfrac{8}{3} + p_1 + 4p_2)n. \tag{2}$$

So,

$E(Kf^*(SPC_{n+1})) = E(Kf^*(SPC_n)) + 12U_n^3 + 140n + 70 = E(Kf^*(SPC_n)) + (108 - 12p_1 - 48p_2)n^2 + (172 + 12p_1 + 48p_2)n + 70$.

Since the initial value is $E(Kf^*(SPC_1)) = 2 \times 2 \times 6 \times \frac{1}{2} \times \left(\frac{5}{6} \times 2 + \frac{4}{3} \times 2 + \frac{3}{2}\right) = 70$,

$E(Kf^*(SPC_n)) = (36 - 4p_1 - 16p_2)n^3 + (32 + 12p_1 + 48p_2)n^2 + (2 - 8p_1 - 32p_2)n$.

This completes the proof. ■

A.4 Proof of Theorem 5.1

Proof. Let $Kf^{+}(SPC_{n+1}) = A_4 + B_4 + C_4$, where $A_4 = \sum_{\{u,v\}\subseteq SPC_n}(d(u)+d(v))r(u,v)$; $B_4 = \sum_{v\in SPC_n\backslash\{u_n\}}\sum_{z_i\in H_{n+1}\backslash\{z_1\}}(d(v)+d(z_i))r(v,z_i)$ and $C_4 = \sum_{\{z_i,z_j\}\subseteq H_{n+1}}(d(z_i)+d(z_j))r(z_i,z_j)$.

$$\begin{aligned}A_4 &= \sum_{\{u,v\}\subseteq SPC_n\backslash\{v_n\}}(d(u)+d(v))r(u,v) + \sum_{v\in SPC_n\backslash\{v_n\}}(d_{SPC_{n+1}}(u_n)+d(v))r(u_n,v),\\ &= \sum_{\{u,v\}\subseteq SPC_n\backslash\{v_n\}}(d(u)+d(v))r(u,v) + \sum_{v\in SPC_n\backslash\{v_n\}}\left(d_{SPC_n}(u_n)+2+\right.\\ &\qquad \left.d(v)\right)r(u_n,v),\\ &= Kf^{+}(SPC_n) + 2\sum_{v\in SPC_n} r(u_n,v)\\ &= Kf^{+}(SPC_n) + 2r(u_n|SPC_n).\end{aligned}$$

$$\begin{aligned}B_4 &= \sum_{v\in SPC_n}\sum_{z_i\in H_{n+1}}(d(v)+d(z_i))r(v,z_i) - \sum_{v\in SPC_n}(d(v)+4)r(v,u_n) -\\ &\qquad \sum_{v\in H_{n+1}}(d(v)+4)r(v,z_1),\\ &= \sum_{v\in SPC_n} d(v)[r(v,u_n) + 2\left(r(v,u_n)+\tfrac{5}{6}\right) + 2\left(r(v,u_n)+\tfrac{4}{3}\right) + 2\left(r(v,u_n)+\right.\\ &\qquad \left.\tfrac{3}{2}\right)] + \sum_{v\in SPC_n}[4r(v,u_n) + 4\left(r(v,u_n)+\tfrac{5}{6}\right) + 4\left(r(v,u_n)+\tfrac{4}{3}\right) + 2\left(r(v,u_n)+\right.\\ &\qquad \left.\tfrac{3}{2}\right)] - \sum_{v\in SPC_n} d(v)r(v,u_n) - 4\sum_{v\in SPC_n} r(v,u_n) - \tfrac{35}{3} - 4\times\tfrac{35}{6},\\ &= 5\sum_{v\in SPC_n} d(v)r(v,u_n) + 10r(u_n|SPC_n) + \tfrac{385}{3}n - \tfrac{35}{3}.\end{aligned}$$

$$C_4 = \sum_{i=1}^{6} d(z_i)\left(\sum_{j=1}^{6} r(z_j,z_i)\right) = \frac{35}{6}\times(4+2\times 5) = \frac{245}{3}.$$

Thus, $Kf^{+}(SPC_{n+1}) = Kf^{+}(SPC_n) + 5\sum_{v\in SPC_n} d(v)r(v,u_n) + 12r(u_n|SPC_n) + \frac{385}{3}n + 70$. As $SPC_n(p_1,p_2)$ is a random spiro chain, $r(u_n|SPC_n)$ is a random variable. Denote $U_n^4 := E(r(u_n|SPC_n))$. Then $E(Kf^{+}(SPC_{n+1})) = E(Kf^{+}(SPC_n)) + 5U_n^3 + 12U_n^4 + \frac{385}{3}n + 70$.

In the following, we calculate U_n^2 by considering three possible cases.

Case 1. $SPC_n \to SPC_{n+1}^1$.

$u_n(z_1)$ coincides with y_5 or y_3 (see Figure 2), thus $r(u_n|SPC_n)$ is given by $r(y_5|SPC_n)$ with probability p_1.

Case 2. $SPC_n \to SPC_{n+1}^2$.

$u_n(z_1)$ coincides with y_6 or y_2 (see Figure 2), thus $r(u_n|SPC_n)$ is given by $r(y_6|SPC_n)$ with probability p_2.

Case 3. $SPC_n \to SPC_{n+1}^3$.

$u_n(z_1)$ coincides with y_4 (see Figure 2), thus $r(u_n|SPC_n)$ is given by $r(y_4|SPC_n)$ with probability $p_3 = 1 - p_1 - p_2$. From Case 1, Case 2 and Case 3, we have that

$$U_n^4 = p_1 r(y_5|SPC_n) + p_2 r(y_6|SPC_n) + (1 - p_1 - p_2) r(y_4|SPC_n),$$
$$= p_1\left[r(u_{n-1}|SPC_{n-1}) + \frac{4}{3}(5n-5) + \frac{35}{6}\right] + p_2\left[r(u_{n-1}|SPC_{n-1}) + \frac{5}{6}(5n-5) + \frac{35}{6}\right] + (1 - p_1 - p_2)\left[r(u_{n-1}|SPC_{n-1}) + \frac{3}{2}(5n-5) + \frac{35}{6}\right],$$
$$= p_1(U_{n-1}^4 + \frac{20}{3}n - \frac{5}{6}) + p_2(U_{n-1}^4 + \frac{25}{6}n + \frac{5}{3}) + (1 - p_1 - p_2)(U_{n-1}^4 + \frac{15}{2}n - \frac{5}{3}),$$
$$= U_{n-1}^4 + (\frac{15}{2} - \frac{5}{6}p_1 - \frac{10}{3}p_2)n + (\frac{5}{6}p_1 + \frac{10}{3}p_2 - \frac{5}{3}).$$

And the initial value is $U_1^4 = r(u_1|SPC_1) = \frac{35}{6}$. Thus,

$$U_n^4 = (\frac{15}{4} - \frac{5}{12}p_1 - \frac{5}{3}p_2)n^2 + (\frac{5}{12}p_1 + \frac{5}{3}p_2 + \frac{25}{12})n.$$

From Equation 2,

$$U_n^3 = (9 - p_1 - 4p_2)n^2 + (\frac{8}{3} + p_1 + 4p_2)n.$$

We have

$$E\big(Kf^+(SPC_{n+1})\big) = E\big(Kf^+(SPC_n)\big) + 5U_n^3 + 12U_n^4 + \frac{385}{3}n + 70,$$
$$= E\big(Kf^+(SPC_n)\big) + (90 - 10p_1 - 40p_2)n^2 + \left(\frac{500}{3} + 10p_1 + 40p_2\right)n + 70.$$

Since the initial value is $E\big(Kf^+(SPC_1)\big) = 70$, so

$$E\big(Kf^+(SPC_n)\big) = \left(30 - \frac{10}{3}p_1 - \frac{40}{3}p_2\right)n^3 + (115 + 10p_1 + 40p_2)n^2 + \left(\frac{5}{3} - \frac{20}{3}p_1 - \frac{80}{3}p_2\right)n$$

This completes the proof. ■

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