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Characterizing Graphs with Nullity $n-4$

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Abstract

The nullity of a graph G, denoted by $\eta(G)$, is the multiplicity of the eigenvalue zero in the spectrum of G. A unified approach is presented for the characterization of graphs of order n with $\eta(G) = n-4$. All known results on trees, unicyclic graphs, bicyclic graphs, graphs with minimum degree 1, and r-partite graphs, for which $\eta(G) = n-4$ are shown to be corollaries of a theorem of Chang, Huang and Yeh that characterizes all graphs with nullity $n-4$.

1 Introduction

Let $G = (V, E)$ be a finite connected simple undirected graph. Its order $|\mathbf{V}|$ and size $|\mathbf{E}|$ are denoted by n and m, respectively. For additional

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graph-theoretic terminology and notation we refer to [3].

The adjacency matrix $\mathbf{A}(G)$ of a graph G with $\mathbf{V} = \{v_1, v_2, \ldots, v_n\}$ is the $n \times n$ matrix (a_{ij}) whose elements are unity if $v_i v_j \in \mathbf{E}(G)$, and zero otherwise.

The eigenvalues of $\mathbf{A}(G)$ form the spectrum of G [10]. The nullity $\eta(G)$ is the algebraic multiplicity of the number zero in the spectrum of G. This spectral feature (having significant chemical applications, see below) was much studied in the mathematical literature, see e.g. [4,6,11,17,18,20,21] and the reviews [1, 13]. Yet, the main problem in this field is unsolved. Namely, until now, in the general case the answer to the fundamental question: "*Given a graph G, what is its nullity?*" is not known. Even worse, in the general case we cannot decide whether a graph is singular ($\eta = 0$) or non-singular ($\eta > 0$). Of course, by calculating the spectrum of G (using any of the available computer-based numerical routines), the above question is easily answered for any particular graph. Also, an algorithm for direct determination of the η-value has been proposed [22].

In chemistry, within the Hückel molecular orbital theory, the nullity of molecular graphs of so called "alternant conjugated hydrocarbons" (which necessarily are bipartite) plays an outstanding role. Namely, η is equal to the number of non-bonding molecular orbitals, and is thus an indicator of stability of the respective chemical compound: $\eta = 0$ is a necessary (but not sufficient) condition for chemical stability. If $\eta > 0$, then the respective species is extremely reactive and usually does not exist; for details see in [9,12]. For this reason, when spectral graph theory started to be applied in chemistry, the first topic to be investigated was nullity [6–9].

For chemical applications, it is of interest to characterize the (molecular) graphs for which $\eta = 0$, $\eta = 1$, and $\eta = 2$. For many classes of molecular graphs (in particular, benzenoid systems and chemical trees) the η-values can be directly determined from the structure of the underlying graph. However, in the general case, this cannot be done. Therefore, it seems natural to try to characterize the graphs for which $n - \eta = k$ for some small values of k. For $k = 0, 1, 2, 3$ this happens to be trivially easy:

Remark.
(a) The only graph G of order n for which $n-\eta=0$ is the edgeless graph, $G \cong \overline{K}_n$.
(b) There is no graph for which $n-\eta=1$.
(c) The only graphs G of order n for which $n-\eta=2$ are the complete bipartite graphs, $G \cong K_{a,b}$, $a+b=n$.
(d) The only graph G of order n for which $n-\eta=3$ is the graph consisting of a triangle and $n-3$ isolated vertices, $G \cong K_3 \cup \overline{K}_{n-3}$.

The first non-trivial case is encountered at $n-\eta=4$, i.e., $\eta=n-4$. In the present paper we are concerned with such graphs.

Chang et al. [2] obtained the following characterization of graphs of order n with nullity $n-4$, or, equivalently, with rank 4.

Definition 1. Let G be a graph with $\mathbf{V}(G)=\{v_1,v_2,\dots,v_n\}$. Let $\mathbf{m}=(m_1,m_2,\dots,m_n)$ be a vector of positive integers. The graph obtained from G by replacing each vertex v_i with an independent set $\{v_i^1,v_i^2,\dots,v_i^{m_i}\}$ and joining v_i^s with v_j^t if and only if $v_iv_j \in \mathbf{E}(G)$ is denoted by $G \circ \mathbf{m}$. This graph is said to be obtained from G by multiplication of vertices.

Theorem 1. *Let G be a connected graph of order n. Then $r(G)=4$ (or equivalently $\eta(G)=n-4$) if and only if G can be obtained from one of the graphs given in Figure 1 by multiplication of vertices.*

Another characterization of graphs with $\eta(G)=n-4$ is given in [5].

In this paper we prove that results on trees with $\eta=n-4$ [16], graphs with $\delta=1$ and $\eta(G)=n-4$ [16], unicyclic graphs with $\eta(G)=n-4$ [19], bicyclic graphs with $\eta(G)=n-4$ ([14] and [15]), and characterization of graphs with $\eta(G)=n-4$ given in [5] can be deduced as corollaries to Theorem 1.

2 Main Results

We use the following notation given in [2]. Let $\mathcal{F}=\{G_1,G_2,\dots,G_k\}$. We denote by $\mathcal{M}(G_1,G_2,\dots,G_k)$ the class of all graphs that can be obtained from one of the graphs in $\{G_1,G_2,\dots,G_k\}$ by multiplication of vertices.

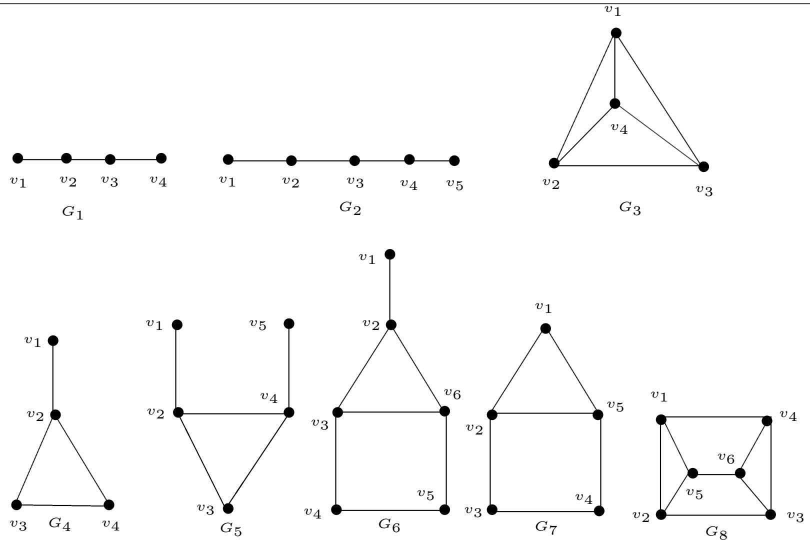

Figure 1. Graphs considered in Theorem 1

It follows from Theorem 1 that $\mathcal{M}(G_1, G_2, \ldots, G_8) = \{G : |\mathbf{V}(G)| = n$ and $\eta(G) = n - 4\}$ where $G_1, G_2, \ldots, G_8$ are the graphs depicted in Figure 1.

Theorem 2. [16] *Let T be a tree of order n and $T \ncong K_{1,n-1}$. Then $\eta(T) = n - 4$ if and only if T is isomorphic to T_1 or T_2, where T_1 and T_2 are shown in Figure 2.*

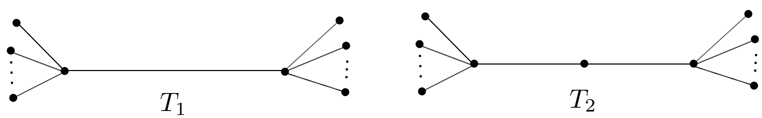

Figure 2. Trees with $\eta(T) = n - 4$; cf. Theorem 2.

Proof. A tree T is in $\mathcal{M}(G_1, G_2, \ldots, G_8)$ if and only if $T \cong P_4 \circ \mathbf{m}$ or $P_5 \circ \mathbf{m}$ where $\mathbf{m} = (m_1, 1, 1, m_4)$ or $(m_1, 1, 1, 1, m_5)$. Clearly $P_4 \circ \mathbf{m}$ is T_1 and $P_5 \circ \mathbf{m}$ is T_2 and hence the result follows. ■

Theorem 3. [19] *Let G be a unicyclic graph of order n with $n \geq 5$. Then $\eta(G) = n - 4$ if and only if G is isomorphic to one of the graphs U_1, U_2, U_3, U_4 or U_5 depicted in Figure 3.*

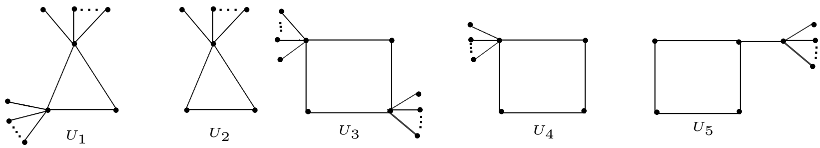

Figure 3. Unicylic graphs with $\eta(G) = n - 4$; cf. Theorem 3.

Proof. A unicyclic graph G is in $\mathcal{M}(G_1, G_2, \ldots, G_8)$ if and only if

$$G \cong \begin{cases} G_4 \circ \mathbf{m} & \text{where } \mathbf{m} = (m_1, 1, 1, 1) \\ G_1 \circ \mathbf{m} & \text{where } \mathbf{m} = (m_1, 1, 2, 1) \\ G_5 \circ \mathbf{m} & \text{where } \mathbf{m} = (m_1, 1, 1, 1, m_5) \\ G_2 \circ \mathbf{m} & \text{where } \mathbf{m} = (m_1, 1, 2, 1, m_5) \\ G_2 \circ \mathbf{m} & \text{where } \mathbf{m} = (1, 2, 1, 1, m_5) \end{cases}$$

$$\begin{aligned} \text{Clearly, } G_4 \circ \mathbf{m} &\cong U_2 \text{ if } \mathbf{m} = (m_1, 1, 1, 1), \\ G_1 \circ \mathbf{m} &\cong U_4 \text{ if } \mathbf{m} = (m_1, 1, 2, 1), \\ G_5 \circ \mathbf{m} &\cong U_1 \text{ if } \mathbf{m} = (m_1, 1, 1, 1, m_5), \\ G_2 \circ \mathbf{m} &\cong U_3 \text{ if } \mathbf{m} = (m_1, 1, 2, 1, m_5) \\ \text{and } G_2 \circ \mathbf{m} &\cong U_5 \text{ if } \mathbf{m} = (1, 2, 1, 1, m_5). \end{aligned}$$

Hence the result follows. ■

Li et al. [15] and Hu et al. [14] independently characterized bicyclic graphs of order n with $\eta(G) = n - 4$. This result has also been reported in the survey paper [13].

Let G be a connected graph of order n and size m. The graph G is said to be bicyclic if $m = n + 1$. Let $\mathcal{B}_n$ denote the set of all bicyclic graphs of order n. The graph obtained from two cycles C_k and C_l by joining a vertex of C_k to a vertex of C_l by a path of length $q-1$ is a bicyclic graph and is denoted by $B(k,q,l)$. Such a graph is called an ∞-graph. A graph consisting of three internally disjoint u-v paths of length l, p, and q, where $l, p, q \geq 1$ and at most one of them is 1, is called a θ-graph and is denoted by $P(l,p,q)$. There are three types of bicyclic graphs. The first type, denoted by $\mathcal{B}_n^+$, is the set of all graphs obtained from an ∞-graph with trees attached when $q=1$. The second type denoted by $\mathcal{B}_n^{++}$ is the set of all graphs obtained from an ∞-graph with trees attached when $q \geq 2$. The third type, denoted by θ_n, is the set of all graphs obtained from a θ-graph with trees attached.

Then $\mathcal{B}_n = \mathcal{B}_n^+ \cup \mathcal{B}_n^{++} \cup \theta_n$.

Li et al. [15] obtained a characterization of all bicyclic graphs in θ_n with nullity $n-4$ and we now deduce this theorem from Theorem 1.

Theorem 4. *Let G be a bicyclic graph of order n in θ_n. Then $\eta(G) = n-4$ if and only if G is isomorphic to one of the graphs $B_i, 1 \leq i \leq 6$, shown in Figure 4.*

Proof.

$$\begin{aligned} \text{Clearly, } B_1 &\cong G_2 \circ \mathbf{m} \textit{ where } \mathbf{m} = (1,3,1,1,m_5) \\ B_2 &\cong G_2 \circ \mathbf{m} \text{ where } \mathbf{m} = (2,2,1,1,m_5) \\ B_3 &\cong G_1 \circ \mathbf{m} \text{ where } \mathbf{m} = (2,2,1,m_4) \\ B_4 &\cong G_6 \circ \mathbf{m} \text{ where } \mathbf{m} = (m_1,1,1,1,1,1) \\ B_5 &\cong G_5 \circ \mathbf{m} \text{ where } \mathbf{m} = (m_1,1,2,1,m_5) \\ \text{and } B_6 &\cong G_2 \circ \mathbf{m} \text{ where } \mathbf{m} = (m_1,1,3,1,m_5) \end{aligned}$$

Hence the graphs B_1, B_2, B_4, B_5, and B_6 have nullity $n-4$.

Since G_8 and G_3 have more than two vertices of degree 3, no graph in θ_n can be obtained by multiplying the vertices of G_3 and G_8.

Since G_7 is a θ-graph, the only graph in θ_n that can be generated from G_7 is by attaching a tree.

Hence the only graph of nullity $n-4$ that can be obtained from G_6 or G_7 by multiplication of vertices is B_4.

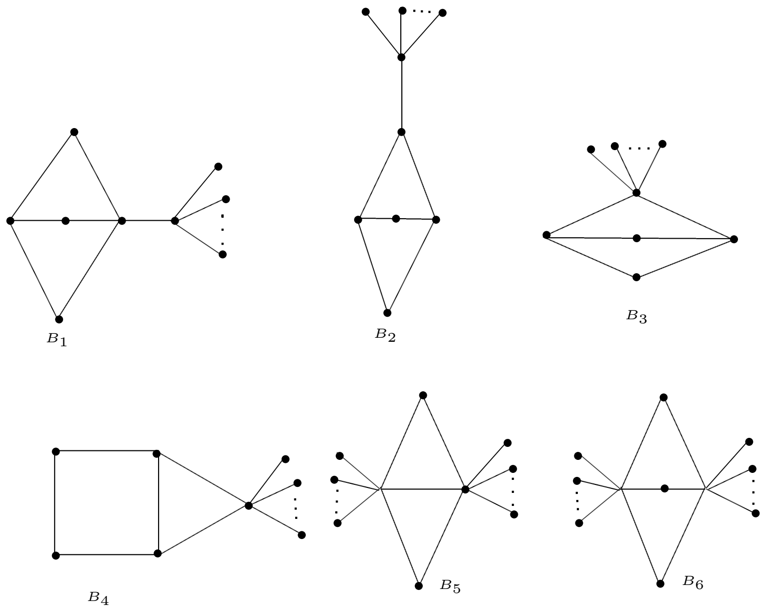

Figure 4. Bicyclic graphs with $\eta = n - 4$; cf. Theorem 4.

The only graph in θ_n that can be generated from G_5 by multiplication of vertices is B_5.

The only graph in θ_n that can be generated by multiplying the vertices of G_4 is the graph depicted in Figure 5. This is included in B_5.

From G_1, the only θ-graph that can be generated by multiplication of vertices is B_3.

Similarly B_2, B_6, and B_7 are the only θ-graphs that can be generated from G_2 by multiplication of vertices.

Hence the theorem follows. ■

Li [16] obtained a characterization of connected graphs of order n with minimum degree $\delta = 1$ having $\eta(G) = n - 4$. These results have also been mentioned in the survey paper [13].

Let G_1^* be a graph of order n obtained from $K_{r,s}$ and $K_{1,t}$ by identifying a vertex of $K_{r,s}$ with the center of $K_{1,t}$, where $r, s, t \geq 1$ and $r + s + t = n$. Let G_2 be a graph of order n obtained from $K_{1,l,m}$ and $K_{1,p}$ by identifying

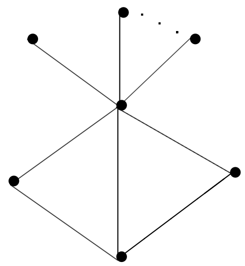

Figure 5. The graph $G_4 \circ \mathbf{m}$ where $\mathbf{m} = (m_1, 1, 2, 1)$; cf. the proof of Theorem 4.

a vertex v of maximum degree in $K_{1,l,m}$ with the center of $K_{1,p}$, where $l, m, p \geq 1$ and $l + m + p + 1 = n$.

The graphs G_1^* and G_2 are dispalyed in Figure 6.

Theorem 5. [16] *Let G be a connected graph of order n with pendent vertices. Then $\eta(G) = n - 4$ if and only if G is isomorphic to the graph G_1^* or G_2^*, where G_2^* is a connected spanning subgraph of G_2 and contains $K_{l,m}$ as its subgraph.*

Proof. Denote by $\mathbf{N}(v)$ the set of vertices adjacent to the vertex v. The graph G_1^* is isomorphic to $P_4 \circ \mathbf{m}$ where $\mathbf{m} = (m_1, 1, r, s-1)$. Let G_2^* be any connected spanning subgraph of G_2 containing $K_{l,m}$ as a subgraph with partite sets $\mathbf{V}_1, \mathbf{V}_2$ and let $|\mathbf{V}_1| = l$ and $|\mathbf{V}_2| = m$. If $|\mathbf{N}(v) \cap \mathbf{V}_1| = l'$ and $|\mathbf{N}(v) \cap \mathbf{V}_2| = m'$, then G_2^* is isomorphic to $G_6 \circ \mathbf{m}$ where $\mathbf{m} = (m_1, 1, m', l - l', m - m', l')$. Hence $\eta(G) = n - 4$ if G is isomorphic to G_1^* or G_2^*.

Conversely, let G be a connected graph of order n with $\delta = 1$ and $\eta(G) = n - 4$. Since $\delta = 1$, G can be obtained from one of the graphs G_1, G_2, G_4, G_5, or G_6 by multiplying the vertices. Since $\delta = 1$, at least one coordinate in $\mathbf{m}$ corresponding to a support vertex must be 1.

Hence for G_1 , $\mathbf{m} = (m_1, 1, m_3, m_4)$ or $(m_1, m_2, 1, m_4)$. If $\mathbf{m} = (m_1, 1, m_3, m_4)$, then $G_1 \circ \mathbf{m}$ is isomorphic to G_1^* where $r = m_3, s = m_4 + 1, t = m_1$. The proof is similar if $\mathbf{m} = (m_1, m_2, 1, m_4)$.

For G_2 either $m_2 = 1$ or $m_4 = 1$. Without loss of generality let $\mathbf{m} = (m_1, 1, m_3, m_4, m_5)$. Then $G_2 \circ \mathbf{m}$ is isomorphic to G_2^* where $l =$

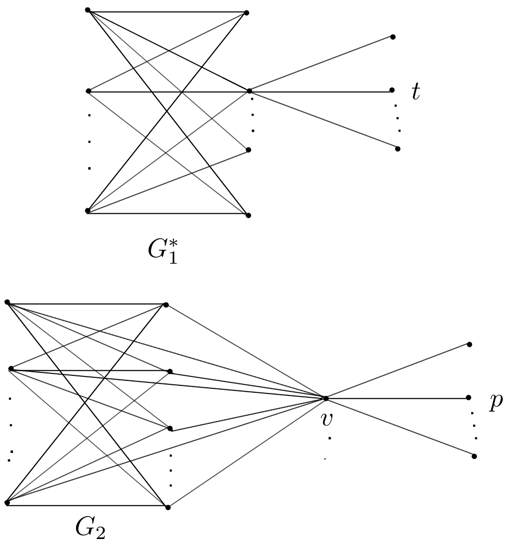

Figure 6. The graphs G_1^* and G_2, mentioned in Theorem 5.

$m_4, m = m_3 + m_5$ and $p = m_1$.

For G_4, $m_2 = 1$. Let $\mathbf{m} = (m_1, 1, m_3, m_4)$. Then $G_4 \circ \mathbf{m}$ is isomorphic to G_2 with $l = m_3, m = m_4$ and $p = m_1$.

For G_5, either $m_2 = 1$ or $m_4 = 1$. Without loss of generality, let $\mathbf{m} = (m_1, 1, m_3, m_4, m_5)$. Then $G_5 \circ \mathbf{m}$ is isomorphic to G_2^* where $l = m_4, m = m_3 + m_5$ and $p = m_1$.

For $G_6, m_2 = 1$. Let $\mathbf{m} = (m_1, 1, m_3, m_4, m_5, m_6)$. Then $G_6 \circ \mathbf{m}$ is isomorphic to G_2^* where $l = m_4 + m_5, m = m_3 + m_6$ and $p = m_1$.

Thus in all cases G is isomorphic to G_1^* or G_2^* and the proof is complete. ■

Another characterization of graphs with $\eta(G) = n - 4$ is given in [5]. The proof of this theorem is tedious and is based on a sequence of ten lemmas. We now prove that this result too is a corollary of Theorem 1.

Let G be an r-partite graph with partite sets $\mathbf{X}_1, \mathbf{X}_2, \ldots, \mathbf{X}_r$ where $r \geq 2$. Let $|\mathbf{X}_i| = m_i$.

Definition 2. A chain-like r-partite graph is a simple r-partite graph with partition $(\mathbf{X}_1, \mathbf{X}_2, \ldots, \mathbf{X}_r)$ in which each vertex of $\mathbf{X}_i$ is joined to each vertex of $\mathbf{X}_{i+1}$ for $i = 1, 2, \ldots, r-1$. This graph is denoted by $P_{m_1,m_2,\ldots,m_r}$ where $|\mathbf{X}_i| = m_i$. For $r \geq 4$, $P^{(1)}_{m_1,m_2,\ldots,m_r}$ is the graph obtained from $P_{m_1,m_2,\ldots,m_r}$ by joining each vertex of $\mathbf{X}_2$ to each vertex of $\mathbf{X}_4$. For $r \geq 5$, the graph $P^{(2)}_{m_1,m_2,\ldots,m_r}$ is the graph obtained from $P_{m_1,m_2,\ldots,m_r}$ by joining each vertex of $\mathbf{X}_1$ to each vertex of $\mathbf{X}_4$ and $\mathbf{X}_5$. For $r \geq 6$, the graph $P^{(3)}_{m_1,m_2,\ldots,m_r}$ is the graph obtained from $P^{(2)}_{m_1,m_2,\ldots,m_r}$ by joining each vertex of $\mathbf{X}_6$ to each vertex of $\mathbf{X}_2$ and $\mathbf{X}_3$.

Theorem 6. [5] *Let G be a connected graph of order n with $n \geq 4$. Then $\eta(G) = n - 4$ if and only if G is isomorphic to $K_{m_1,m_2,\ldots,m_r} (r = 4)$, $P_{m_1,m_2,\ldots,m_r}$ $(r = 4$ or $r = 5)$, $P^{(1)}_{m_1,m_2,\ldots,m_r}$ $(r = 4$ or $r = 5)$, $P^{(2)}_{m_1,m_2,\ldots,m_r}$ $(r = 5$ or $r = 6)$ or $P^{(3)}_{m_1,m_2,\ldots,m_r}$ $(r = 6)$, where $m_1 + m_2 + \cdots + m_r = n$ and $m_i > 0$ for all $i = 1, 2, \ldots, r$.*

Proof. Let $\mathbf{m} = (m_1, m_2, \ldots, m_r)$. Then $K_{m_1,m_2,\ldots,m_r}(r = 4)$ is isomorphic to $G_3 \circ \mathbf{m}$. The graph $P_{m_1,m_2,\ldots,m_r}(r = 4$ or $r = 5)$ is isomorphic to $G_1 \circ \mathbf{m}$ or $G_2 \circ \mathbf{m}$. The graph $P^{(1)}_{m_1,m_2,\ldots,m_r}$ $(r = 4$ or $r = 5)$ is isomorphic to $G_4 \circ \mathbf{m}$ or $G_5 \circ \mathbf{m}$. The graph $P^{(2)}_{m_1,m_2,\ldots,m_r}$ $(r = 5$ or $r = 6)$ is isomorphic to $G_7 \circ \mathbf{m}$ or $G_6 \circ \mathbf{m}$. The graph $P^{(3)}_{m_1,m_2,\ldots,m_r}$ $(r = 6)$ is isomorphic to $G_8 \circ \mathbf{m}$. Hence the result follows. ■

3 Conclusion

We have presented an unified approach for the characterization of graphs of order n with nullity $n - 4$. A similar approach for graphs with nullity $n - 5$ and $n - 6$ can be carried out and results in this direction will be presented in a subsequent paper.

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