Spectral Theory of Graphs in Chemistry. 1. Projection Operators and Canonical Numeration of Graph Vertices

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An algorithm for the construction of canonical numeration of graph vertices for any labeled graph based on the usage of projection operators is described. Some examples are considered.

1. INTRODUCTION

Spectral characteristics of graphs are widely used in various sections of the graph theory, theoretical physics, theoretical chemistry, and other fields of science.[1-8] The given work shows in what way some of such values can be used for canonical numeration of vertices of an arbitrary graph. The given method is illustrated by a number of examples.

The question of canonical numeration of graph vertices is considered in mathematical and chemical literature in connection with the problems of graph isomorphism and coding of structure formulas of chemical compounds. These problems appear, for example, in the course of searching for a compound in a data base or in computer-assisted synthesis. The literature contains various descriptions of canonical numerations of graph vertices as well as methods of ordering of atoms or functional groups in chemical compounds.[6-22] Most of these methods deal with the partitioning of the vertices belonging to the molecular graph (MG) or a graph of a more common type into equivalence classes. For this purpose usually vertex invariants of MG are used, which are calculated in terms of various structural characteristics of MG, such as vertex degrees, numbers of the neighbors of the first, second, or higher orders, components of the main eigenvector of the adjacency matrix, and several others (see, for example, refs 9, 10, and 15–18). A number of canonization algorithms of the adjacency matrix of a simple graph are based on the vertex ordering procedure, which leads to the adjacency matrix corresponding to the minimum or maximum binary code.[12,13,20]

The given work presents an algorithm of canonization based on the usage of vertex and edge spectral type invariants of MG. These invariants are built in a definite way with the help of the elements of the projection operators on certain invariant subspace of the adjacency matrix. An algorithm can be applied to an arbitrary weighted graph and alongside with canonical numeration of vertices makes it possible to find elements of an automorphism group of MG.

2. CANONIZATION PROCEDURE

Let G_n be the labeled graph with the vertices $v_1,...,v_n$, adjacency matrix $\mathbf{A}(G_n)$, eigenvalues λ_j, eigenvectors $\bar{c}_j = (c_{j1},...,c_{jn})$ $(j = 1,...,n)$, and spectrum $\Sigma = \{\sigma_1,...,\sigma_m\}$, $\lambda_1 \geq \lambda_2 \geq ... \geq \lambda_n$, $\sigma_1 > \sigma_2 > ... > \sigma_m$. Let $P_n^{(\sigma_j)} = \|P_{kl}^{(\sigma_j)}\|$ to denote the projection operator on invariant subspace of the matrix $\mathbf{A}(G_n)$, corresponding to the spectrum point σ_j; $P_{kl}^{(\sigma_j)} = \sum_t c_{tk}c_{tl}$, and the sum is distributed on eigenvectors $\bar{c}_t$, for which $\lambda_t = \sigma_j$.

It should be noted that diagonal elements of projectors $P_n^{(\sigma_j)}$, $\bar{P}_n^{(\sigma_j)} \equiv (P_{11}^{(\sigma_j)},...,P_{nn}^{(\sigma_j)})$ are vertex invariants, and nondiagonal elements $P_{kl}^{(\sigma_j)}$ $(k \neq l, \sigma_j \in \Sigma)$ are edge invariants. Hence, one can use their values for partition of the vertices $v_1,...,v_n$ into ordered equivalence classes. The suggested algorithm consists of three main steps.

1. *The calculation of eigenvalues, eigenvectors, and projectors with the help of standard computer programs.*

2. *The vertex ordering on the basis of the vectors* $\bar{A}_i = (P_{ii}^{(\sigma_1)},...,P_{ii}^{(\sigma_m)})$. Let us assume that $v_i \leq v_j$, if $\bar{A}_i \leq \bar{A}_j$ in a lexicographical sense. As a result the vertex set $\{v_1,...,v_n\}$ will be divided into ordered equivalence classes, some of which will contain more than one vertex. For all vertices belonging to such a class, diagonal elements of projectors $P^{(\sigma_k)}$ are equal (for all $\sigma_k \in \Sigma$). It is known that such vertices of MG are isospectral.[23] Two vertices v_i and v_j of graph G are called isospectral ones, if for any graph H the graphs $(G + H)_i$ and $(G + H)_j$ have one and the same spectrum. The graph $(G + H)_i$ (or $(G + H)_j$) is constructed from G and H in the following way: the vertex v_i or v_j is connected by an edge with a fixed vertex of H.[23]

3. *The ordering of isospectral vertices on the basis of the values* $P_{ij}^{(\sigma_k)}$ $(i \neq j)$, $\sigma_k \in \Sigma$. Suppose that all vertices of the first r equivalence classes are ordered, and they have old numbers $j_1,...,j_N$ and new numbers 1,...,N. It is required to order the vertices $v_{i_1},...,v_{i_L}$ from the $(r + 1)$th class relative to vertices $v_{j_1},...,v_{j_N}$. This task is solved by comparison of the vectors $\bar{Y}_{i_1}^{(\sigma)} = (P_{i_1j_N}^{(\sigma)},...,P_{i_1j_1}^{(\sigma)}),...,\bar{Y}_{i_L}^{(\sigma)} = (P_{i_Lj_N}^{(\sigma)},...,P_{i_Lj_1}^{(\sigma)})$ $(\sigma \in \Sigma)$: if $\bar{Y}_{i_a}^{(\sigma)} \leq \bar{Y}_{i_b}^{(\sigma)}$ in lexicographical sense, then $v_{i_a} \leq v_{i_b}$. If for two vertices v_{i_a} and v_{i_b} $\bar{Y}_{i_a}^{(\sigma)} \equiv \bar{Y}_{i_b}^{(\sigma)}$ for some value $\sigma = \sigma_k$, then one should turn to the next value $\sigma = \sigma_{k+1}$. If for each j $(j_1 \leq j \leq j_N)$ and $\sigma \in \Sigma$ the vertices of the $(k+1)$th class cannot be ordered, then it may be that there are several numerations for these vertices, and all possible numerations are necessary to consider. For this purpose an arbitrary vertex from the

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$(k+1)$th class is initially chosen (for example, i_1), and for ordering of another vertices the values $P_{ij}^{(\sigma)}$ ($i = i_1$, $j \in \{i_2,...,i_L\}$, $\sigma \in \Sigma$) should be compared. (If $P_{i_1a}^{(\sigma)} \le P_{i_1b}^{(\sigma)}$ then $v_a \le v_b$.) Then all other vertices should be considered as the first elements.

Suppose that the first equivalence class consists of more than one vertex. In this case the ordering procedure begins with the choice of the first element in this class. For the ordering of another vertices the procedure described above is used.

Suppose that several numerations of graph vertices are received as a result of the described above procedure. To each numeration corresponds the adjacency matrix. If these matrices are different, then as the canonical matrix one should take the one which, when written in one line, is bigger in the lexicographical sense. Numerations corresponding to it will be canonical numerations. The number of such numerations does not exceed the order of the automorphism group of the graph, and to each pair of numerations corresponds a nontrivial group element.

3. REMARKS

1. When investigating the electron structure of conjugated molecules by such methods of quantum chemistry as that of Huckel, Pariser–Parr–Pople, etc., the eigenvalues and eigenvectors of some matrices are usually calculated. Hence in these cases the proposed algorithm can be used without any additional calculations for ordering of the results of quantum chemical calculations and for compiling the corresponding data bases.

2. For the solution of the canonization problem in some cases the projector $P^+ = \sum_{\sigma_j \ge 0} P^{(\sigma_j)}$ can be used instead the projectors $P^{(\sigma_j)}(j = \overline{1,m})$. The results of both procedures will be identical. The matrix $\mathbf{P}^+$ is easy to find approximately without the calculation of eigenvalues and eigenvectors: $\mathbf{P}^+ = \mathbf{E} + \mathbf{A}|\mathbf{A}|$, where $\mathbf{E}$ is the identity matrix, $|\mathbf{A}|$ is the module function of $\mathbf{A}$, $|\mathbf{A}| \approx a_0 + a_2\mathbf{A}^2 + ... + a_{2k}\mathbf{A}^{2k} + ...$ The numbers a_i ($i = 0,2,...,2k$) are taken from the presentation $|X| \approx a_0 + a_2X^2 + ... + a_{2k}X^{2k} + ...$ ($|X| \le \lambda_1$, $\lambda_1 \le 4$ for chemical nonweighted graphs).[24]

3. For bipartite graphs the elements of $P^{(\lambda_j)}$ ($\lambda_j < 0$) are expressed through the elements of $P^{(\lambda_j)}$ ($\lambda_j > 0$). Hence, for such graphs a canonization procedure deals with the projectors $P^{(\lambda_j)}$ ($\lambda_j \ge 0$) only.

4. For regular graphs $P_{ij}^{(\lambda_1)} = 1/n(i,j = \overline{1,n})$, hence for the purpose of vertex classification the projector $P^{(\lambda_1)}$ is useless.

5. It is known that maximal eigenvalue λ_1 of MG is simple, and components of corresponding eigenvector $\bar{c}_1 = (c_{11},...,c_{1n})$ may be chosen positive.[25] From the relation $\bar{P}_n^{(\sigma_1)} = (c_{11}^2,...,c_{1n}^2)$ is followed that partitioning the vertices into classes using components of $P_n^{(\sigma_1)}$ and $\bar{c}_1$ give one and the same result. Hence for vertex classification the values c_{1i} instead of the values $P_{ii}^{(\sigma_1)}$ ($i = \overline{1,n}$) may be used.

4. EXAMPLES

1. Let us consider molecular graph G_6 describing the carbon skeleton of a benzene molecule (Figure 1). Its eigenvalues are of the numbers $\{2,1,1,-1,-1,-2\}$, and its spectrum is the set $\Sigma = \{2,1,-1,-2\}$. But due to the fact that graph G_6 is a bipartite one, elements of $P^{(-\sigma_i)}$ are expressed through the elements of $P^{(\sigma_i)}$, $\sigma_1 = 1,2$. As graph G_6 is regular of the second degree one, all elements of $P^{(2)}$ are equal and all vertices of G_6 are isospectral. Hence further consideration deals with

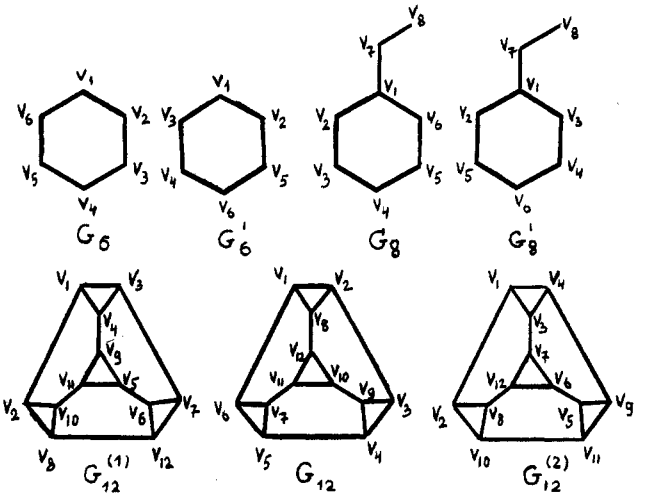

Figure 1. Graphs G_6, G_8, and G_{12}. Canonical numerations of their vertices are given on graphs G_6', G_8', $G_{12}^{(1)}$, and $G_{12}^{(2)}$, correspondingly.

operator $P^{(1)}$ only, designated through $\mathbf{P}$. This operator has the following form:

$$\mathbf{P} = \|P_{ij}\| = \begin{Vmatrix} 2p & p & -p & -2p & -p & p \\ p & 2p & p & -p & -2p & -p \\ -p & p & 2p & p & -p & -2p \\ -2p & -p & p & 2p & p & -p \\ -p & -2p & -p & p & 2p & p \\ p & -p & -2p & -p & p & 2p \end{Vmatrix}$$

where $p = 1/6$.

Let us choose vertex v_1 as the first one. With the help of the first line, elements of matrix $\mathbf{P}$ partition vertices $v_2,v_3,...,v_6$ into equivalence classes relative to the vertex v_1 in accordance with the values of elements P_{1j} (if $P_{1j_1} \ge P_{1j_2}$ then $v_{j_1} \ge v_{j_2}$). Three equivalence classes are received as the result: $\{v_2,v_6\}$, $\{v_3,v_5\}$, and $\{v_4\}$. But positions of vertices v_3 and v_5 relative to the vertices of class $\{v_2,v_6\}$ are different, what follows from inequalities $P_{2,3} > P_{2,5}$ and $P_{6,5} > P_{6,3}$. Besides, as the first vertex in the class $\{v_2,v_6\}$ may be chosen the vertex v_2 or v_6. The use of inequalities for elements P_{ij} as a criterion of ordering within the limits of one and the same class will result in two numerations v_1,v_2,v_6,v_5,v_3,v_4 (see Figure 1, graph G_6') and v_1,v_6,v_2,v_3,v_5,v_4. It is not difficult to check that these two sequences lead to one and the same adjacency matrix. Hence, vertices v_2,v_6 and v_2,v_5 are equivalent in the theoretical group sense. These two methods of ordering generate the permutation (1)(2,6)(3,5)(4) which is the element of the graph group.

Next, choose vertex v_2 as the initial one and carry out the analogous procedure. Then repeat the procedure with vertices v_3, v_4, etc. Each time one and the same adjacency matrix is received. As an additional result we find elements of a graph group (1,2,3,4,5,6), (1)(2,6)(3,5)(4), (2)(1,3)(4,6)(5), and (3)(2,4)(1,5)(6), which can easily make up a graph group taking into account the identity element (1)(2)(3)(4)(5)(6).

2. Let us consider graph G_8, describing the carbon skeleton of a styrene molecule (Figure 1). The graph G_8 is a bipartite one; its spectrum is simple and does not contain zero. Hence all spectral characteristics of this graph can be expressed in terms of positive eigenvalues and eigenvectors corresponding to them. All these values for G_8 are given in Table 1.

On the basis of analysis of the squares of components c_{ij} of eigenvectors $\bar{c}_i = (c_{i1},...,c_{in})$ partition the graph vertices into the following equivalence classes $\{v_1\}$, $\{v_2,v_6\}$, $\{v_3,v_5\}$, $\{v_4,v_7\}$, and $\{v_8\}$. Classes are arranged in decreasing order of values $(c_{ij})^2$. In the given case there are three pairs of isospectral

Table 1. Positive Eigenvalues λ_l and Components c_{ij} for Corresponding Eigenvectors C_l of Graph G_8

	λ_l			
C_l	2.13	1.41	1.00	0.66
1	0.513	0.353	0.000	–0.334
2	0.394	0.000	0.500	–0.307
3	0.328	–0.353	0.500	0.130
4	0.307	–0.500	0.000	0.394
5	0.328	–0.353	–0.500	0.130
6	0.394	0.000	–0.500	–0.307
7	0.307	0.500	0.000	0.394
8	0.144	0.353	0.000	0.595

Table 2. Matrix Elements $P_{ij}^{(+)}$ of Operator $P^{(+)}$ of Graph G_{12}

	1	2	3	4	5	6	7	8	9	10	11	12
1	1.00											
2	0.42	1.00										
3	–0.08	0.67	1.00									
4	–0.25	–0.08	0.42	1.00								
5	–0.08	–0.25	–0.08	0.67	1.00							
6	0.67	–0.08	–0.25	–0.08	0.42	1.00						
7	–0.08	0.17	0.17	–0.08	0.42	0.42	1.00					
8	0.42	0.42	–0.08	0.17	0.17	–0.08	–0.25	1.00				
9	0.17	–0.08	0.42	0.42	–0.08	0.17	–0.25	–0.25	1.00			
10	0.17	–0.25	–0.08	–0.08	–0.25	0.17	–0.08	–0.08	0.67	1.00		
11	–0.25	0.17	0.17	–0.25	–0.08	–0.08	0.67	–0.08	–0.08	0.42	1.00	
12	–0.08	–0.08	–0.03	0.17	0.17	–0.25	–0.08	0.67	–0.08	0.42	0.42	1.00

vertices $\{v_4,v_7\}$, $\{v_3,v_5\}$, and $\{v_2,v_6\}$. Let us order the vertices in these classes in the following way.

Since vertices v_2 and v_6 are equivalent relative to v_1 ($P_{1,6}^{(\sigma)} = P_{1,2}^{(\sigma)}$ for all $\sigma \in \Sigma$), then two different ways of ordering these two vertices are possible. Then consider vertices v_3 and v_5. These vertices are not equivalent neither relative to v_2 nor relative to v_6, as $P_{3,2}^{(1)} = 0.25$, $P_{5,2}^{(1)} = -0.25$, $P_{6,2}^{(1)} = -0.25$, and $P_{6,5}^{(1)} = 0.25$. Vertices v_4 and v_7 are equivalent relative to each vertex of the classes $\{v_2,v_6\}$ and $\{v_3,v_5\}$. But vertices v_4, v_7 are distinctly relative to v_1 as $P_{1,4}^{(1,4)} < P_{1,7}^{(1,4)}$.

Hence, there are only two methods of ordering vertices which are possible in the given case (see Figure 1, graph G_8'):

$$v_1, v_2, v_6, v_5, v_3, v_4, v_7, v_8$$

$$v_1, v_6, v_2, v_3, v_5, v_4, v_7, v_8$$

It is not difficult to check that both methods of ordering lead to one and the same adjacency matrix and generate permutation of vertices, which is an element of the graph group.

3. Let us consider the graph G_{12} describing a truncated tetrahedron (Figure 1). Its eigenvalues are the numbers {3;2,2,2;0,0,–1,–1,–1,–2,–2,–2}, and its spectrum is the set Σ = {3,2,0,–1,–2}. All the vertices of graph G_{12} are isospectral. In the given case in order to construct canonical numeration it is sufficient to use projector $P^{(+)} = \sum_{\sigma_i \geq 0} P^{(\sigma_i)}$ on invariant subspace of the adjacency matrix of graph G_{12}, corresponding to its non-negative eigenvalues. The lower triangle of $P^{(+)}$ is given in Table 2. Choose vertex v_1 initially and partition the vertices $v_2,\ldots,v_{12}$ into equivalence classes relative to v_1. Comparing the values of the elements in the first column of matrix $\mathbf{P}^{(+)}$, we find the following classes:

$$\{v_1\},\{v_6\},\{v_2,v_8\},\ \{v_9,v_{10}\},\ \{v_3,v_5,v_7,v_{12}\},\ \{v_4,v_{11}\}$$
$$(0.67)(0.42)\quad (0.17)\quad (-0.08)\quad (-0.25)$$

(Round brackets contain corresponding values of elements $P_{1j}^{(+)}$). Vertices of class $\{v_2,v_8\}$ are not distinct relative to v_6 as well as to v_1. Hence two different numerations of the vertices v_2,v_8 are possible. Then consider class $\{v_9,v_{10}\}$. Vertices v_9 and v_{10} are distinct relative to v_2 as well as relative to v_8: $P_{9,8}^{(+)} = -0.25$; $P_{9,2}^{(+)} = -0.08$; $P_{10,8}^{(+)} = -0.08$; $P_{10,2}^{(+)} = -0.25$. Hence, the numeration of vertices belonging to this class is determined by the order of vertices in the preceding class $\{v_2,v_8\}$.

Let us consider now the following class $\{v_3,v_5,v_7,v_{12}\}$. Vertices v_3 and v_5 are distinct relative to vertices v_9 and v_{10}. Vertices v_7 and v_{12} have analogous property. Corresponding elements of matrix $\mathbf{P}^{(+)}$ are equal to the following values:

$$P_{10,3}^{(+)} = -0.08,\ P_{10,5}^{(+)} = -0.25;\ P_{10,7}^{(+)} = -0.08;\ P_{12,10}^{(+)} =$$
$$0.42;\ P_{9,3}^{(+)} = 0.42;\ P_{9,5}^{(+)} = -0.08;\ P_{9,7}^{(+)} = -0.25;\ P_{9,12}^{(+)} = -0.08$$

Relative to v_{10} the vertex set $\{v_3,v_5,v_7,v_{12}\}$ is partitioned into three such classes:

$$\{v_{12}\},\quad \{v_3,v_7\},\quad \{v_5\}$$
$$(0.42)\quad (-0.08)\quad (-0.25)$$

and relative to v_9 corresponding classes have the following form:

$$\{v_3\},\quad \{v_5,v_{12}\},\quad \{v_7\}$$
$$(0.42)\quad (-0.08)\quad (-0.25)$$

Vertices of the last class $\{v_4,v_{11}\}$ are distinct relative to v_5 and to v_7: $P_{5,4}^{(+)} = 0.67$, $P_{5,11}^{(+)} = -0.08$, $P_{7,4}^{(+)} = -0.08$, $P_{7,11}^{(+)} = 0.67$. Hence, we get two sequences of vertices:

$$v_1, v_6, v_2, v_8, v_{10}, v_9, v_3, \{v_5,v_{12}\}, v_7, v_{11}, v_4$$

$$v_1, v_6, v_8, v_2, v_9, v_{10}, v_{12}, \{v_3,v_7\}, v_5, v_4, v_{11}$$

The vertices v_{12} and v_5 are distinct relative to v_3: $P_{3,12}^{(+)} = -0.25$, $P_{3,5}^{(+)} = -0.08$. Similarly, v_3 and v_7 are not equivalent relative to v_{12}: $P_{12,3} = -0.25$; $P_{12,7} = -0.08$. Taking into consideration these values, we shall finally get two numerations of vertices:

$$v_1, v_6, v_2, v_8, v_{10}, v_9, v_3, v_5, v_{12}, v_7, v_{11}, v_4$$

$$v_1, v_6, v_8, v_2, v_9, v_{10}, v_{12}, v_7, v_3, v_5, v_4, v_{11}$$

These numerations are plotted on graphs, given in Figure 1 (graphs G_{12}' and G_{12}'') and correspond to one and the same adjacency matrix. Further analysis of permissible numerations of the graph is carried out similar to that of graph G_6.

5. SOME RESULTS OF THE COMPUTER ASSISTED CONSTRUCTION OF THE CANONICAL NUMERATION

For testing of the suggested algorithm PASCAL and FORTRAN programs oriented on an IBM PC were elaborated. Using the PASCAL program the canonical numerations for a broad series of graphs represented by the adjacency matrices were constructed. For such programs the computational time is interesting. For example, the computational times (in seconds) for molecular graphs pictured in Figure 2a–j are indicated (in brackets, for step 1 of the algorithm; without brackets, for steps 2 and 3). Graphs 2a–h are taken from ref 26. Using the FORTRAN program we found all elements of the automorphism group of the truncated

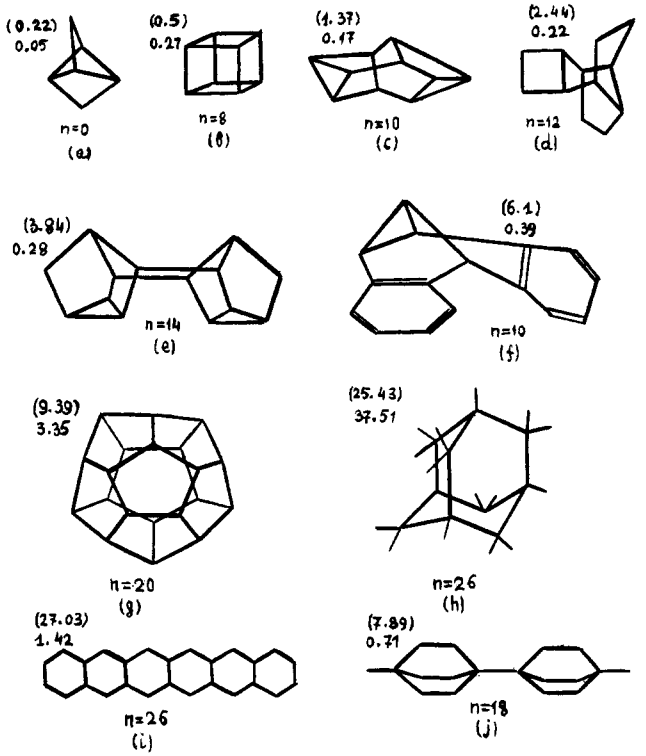

Figure 2. Computation times (for step 1 of the algorithm, in brackets; for steps 2 and 3, without brackets) for several molecular graphs.

icosahedral pure carbon molecule C_{60} in 67 s (IBM PC AT - 386/387). The programs are freely available for interested scientists.

6. CONCLUSIONS

In this article a new method for canonical labelings of graphis is described. The method is based on spectral properties of the adjacency matrices. This method was described briefly in an earlier abstract[27,28] and more completely in ref 29. When the present paper had already been prepared, the article of T. P. Zivkovic,[30] in which analogous problems are discussed, was published.

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