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Graph theoretical study of topologically determined electronic energy levels ☆

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Abstract

In order to find topologically determined electronic energy levels a special partitioning of basis functions is given. General conditions are presented for the existence and non-existence of Sachs graphs. © 2000 Elsevier Science B.V. All rights reserved.

Keywords: Hamiltonian matrices; Graph theoretical study; Sachs graphs

1. Introduction

In our previous papers [1–6] we demonstrated, based on graph theory [7–17], the existence of topologically determined eigenvalues of symmetrical Hamiltonian matrices. These eigenvalues were equal to some diagonal elements of the matrix and were not depending on the actual values of other diagonal and non-zero off-diagonal matrix elements. Such kind of matrices can be found very easily in the study of the electronic structure of molecules and clusters if a tight-binding first neighbor approximation is used. In these matrices the appropriate distribution of $H_{ij} = 0$ zero matrix elements can guarantee the zero value of several determinants that determine the coefficients of the characteristic polynomial (recall that eigenvalues are given as the roots of this polynomials). These special distributions of off-diagonal zero and non-zero matrix elements were described with the help of the non-existence of Sachs graphs [7] of the graph of the Hamiltonian matrix. In practical applications, however, the demonstration of the existence of a special graph structure is much easier than the demonstration of the non-existence of Sachs graphs. In this paper a special graph structure is given that describes the graphs with N vertices which do not have Sachs graphs with N, $(N-1)$,…,$(N-\nu+1)$ vertices. In Section 2 the basic definitions and the relations between matrices and graphs are given. Theorem 1 of Section 3 clarifies when the above mentioned graph structure is met and Theorem 2 shows its general properties. In Section 4 our results are summarized in Theorem 3 without a reference to the special terminology of graph theory.

2. Matrices and graphs

In this paper we shall study the eigenvalue problem of the symmetrical square matrix $H = [H_{ij}]$ of size $N \times N$. The characteristic polynomial $D(\epsilon)$ of H can be written as [18,19]

$$D(\epsilon) = \det|\epsilon I - H| = \sum_{n=0}^{N} a_n \epsilon^{N-n}, \quad (1)$$

where I is the unit matrix and the coefficients of $D(\epsilon)$

☆ Dedicated to Professor R. Gáspár on the occasion of his 80th year.

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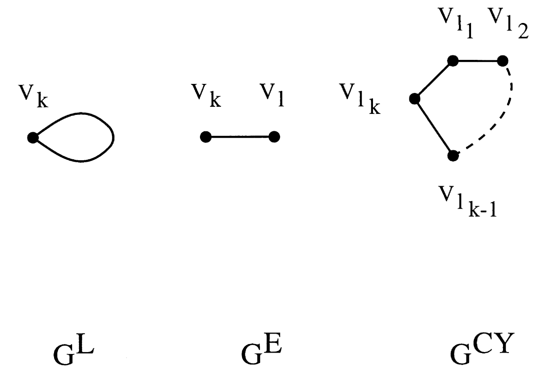

Fig. 1. Loop graph G^L, complete graph with two vertices and one edge G^E, and cyclic graph C^{CY} (see Lemma 1).

are given by

$$a_n = (-1)^n \sum H(i_1 i_2 \ldots i_n), \tag{2}$$

where a summation runs over all

$$\binom{N}{n}$$

principal minors of H of order n. These minors are given by

$$H(i_1 i_2 \ldots i_n) = \sum_{(j_1 j_2 \ldots j_n)} (-1)^{t(p)} H_{i_1 j_1} H_{i_2 j_2} \ldots H_{i_n j_n} \tag{3}$$

where $t(p)$ is the parity of the permutation $j_1 j_2 \ldots j_n$ with respect to the permutation $i_1 i_2 \ldots i_n$.

Definition 1. The graph $G = (V, E)$ is the graph of square matrix $H = [H_{ij}]$ of size $N \times N$ if $V = \{v_1, v_2, \ldots, v_N\}$ is the set of N vertices and $(v_i, v_j) \in E$ if and only if $H_{ij} = H_{ij} \neq 0$. Here E is the set of edges, and (v_i, v_j) is the edge determined by the unordered pair of vertices v_i and v_j.

From Definition 1 follows that the graph G of matrix H is not a directed graph and G does not contain multiple edges. In this paper graph G means always a non-directed graph without multiple edges.

Definition 2. Let $j_1 j_2 \ldots j_n$ be a permutation of numbers $i_1 i_2 \ldots i_n$ with $H_{i_1 j_1} H_{i_2 j_2} \ldots H_{i_n j_n} \neq 0$. Then $G^S = (V^S, E^S)$ is a Sachs graph of G with n vertices if $V^S = \{v_{i_1}, v_{i_2}, \ldots, v_{i_n}\}$ and $E^S = \{(v_{i_1}, v_{j_1}), (v_{i_2}, v_{j_2}), \ldots (v_{i_n}, v_{j_n})\}$. G^S is not a directed graph and multiple edges are not allowed. Thus (v_k, v_l) and (v_l, v_k) mean the same edge.

Lemma 1. *Let* G *be a graph of matrix* H *and let* G^S *be a Sachs graph of graph* G. *Then* G^S *is a subgraph of* G *and the components of* G^S *can only be one or more of the following graphs (Fig. 1):*

1. *Loop graph* $G^L = (V^L, E^L)$, *where* $V^L = \{v_k\}$, $E^L = \{(v_k, v_k)\}$. *The set of* G^L *components of* G^S *is* $C^L(G^S)$.
2. *Complete graph of two vertices and one edge* $G^E = (V^E, E^E)$, *where* $V^E = \{v_k, v_l\}, E^E = \{(v_k, v_l)\}$. *The set of* G^E *components of* G^S *is* $C^E(G^S)$.
3. *Cyclic graph* $G^{CY} = (V^{CY}, E^{CY})$, *where* $V^{CY} = \{v_{l_1}, v_{l_2}, \ldots, v_{l_K}\}$, $E^{CY} = \{(v_{l_1}, v_{l_2}), (v_{l_2}, v_{l_3}), \ldots, (v_{l_{K-1}}, v_{l_K}), (v_{l_K}, v_{l_1})\}$. *The set of* G^{CY} *components of* G^S *is* $C^{CY}(G^S)$.

Proof. From $H_{i_1 j_1} H_{i_2 j_2} \ldots H_{i_n j_n} \neq 0$. follows that $H_{i_1 j_1} \neq 0, H_{i_2 j_2} \neq 0, \ldots, H_{i_n j_n} \neq 0$. Thus G^S is a subgraph of G. The statement concerning the components of G^S follows from the fact that every permutation $j_1 i_2 \ldots j_n$ of numbers $i_1 i_2 \ldots i_n$ can be described as a product of disjunct cycles. The cycle (k, k) corresponds to the loop (v_k, v_k) and the cycle $(k, l)(l, k)$ is represented by the complete graph of edge (v_k, v_l). The other cycles yield the cyclic graphs. □

Lemma 2. *Let* G *be a graph of symmetrical square matrix* H *of size* $N \times N$ *and suppose that* G *does not have Sachs graphs with* N, $N-1$, …, $N-\nu+1$ *vertices. Then* $\epsilon = 0$ *is a* ν*-fold degenerated eigenvalue of* H *(*ν *is an integer).*

Proof. If G does not have Sachs graph with $N, N-1, \ldots, N-\nu+1$ vertices, we obtain that $H_{i_1 j_1} H_{i_2 j_2} \ldots H_{i_n j_n} = 0$ for $n \geq N-\nu+1$ and from Eqs. (1)–(3) follows that

$$a_N = a_{N-1} = a_{N-2} = \cdots = a_{N-\nu+1} = 0. \tag{4}$$

□

Remark 1. *The study of* $\epsilon = H_{kk}$ *eigenvalue can be carried out with the study of* $\epsilon = 0$ *eigenvalue of the matrix* $H' = H - H_{kk}I$ *(Here* I *is the unit matrix).*

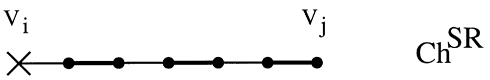

Fig. 2. A reduced chain $\mathrm{Ch}^{\mathrm{SR}}$ between the vertices v_i and v_j; $v_i \notin V(G^{\mathrm{SR}})$ and $v_j \in V(G^{\mathrm{SR}})$. The edges of $C^{\mathrm{E}}(G^{\mathrm{SR}})$ are marked by thick solid line. The edges with thin solid line do not belong to $C^{\mathrm{E}}(G^{\mathrm{SR}})$. The vertex $v_i \notin V(G^{\mathrm{SR}})$ is marked by X (see Definition 5).

3. Study of Sachs graphs

Theorem 1. *Suppose that the* N *vertices of a non-directed graph without multiple edges* $\mathrm{G} = (\mathrm{V}, \mathrm{E})$ *can be partitioned into three disjunct sets* V_1, V_2 *and* V_3 *with the following properties:*

1. *Set* V_1*: If* $\mathrm{v_i} \in \mathrm{V}_1$ *and* $\mathrm{v_j} \in \mathrm{V}_1$ *then* $(\mathrm{v_i}, \mathrm{v_j}) \notin \mathrm{E}$. *Loops are not allowed in* V_1 *and the number of vertices in set* V_1 *is* $\mathrm{m} > 0$.
2. *Set* V_2*: If* $\mathrm{v_{i'}} \in \mathrm{V}_2$ *then there is at least one edge* $(\mathrm{v_{i'}}, \mathrm{v_{j'}}) \in \mathrm{E}$ *with vertex* $\mathrm{v_{j'}} \in \mathrm{V}_1$. *The number of vertices in set* V_2 *is* $\mathrm{n} \geq 0$.
3. *Set* V_3: $\mathrm{v_k} \in \mathrm{V}_3$ *if* $\mathrm{v_k} \notin \mathrm{V}_1$ *and* $\mathrm{v_k} \notin \mathrm{V}_2$. *The number of vertices in set* V_3 *is* $\mathrm{N} - \mathrm{m} - \mathrm{n} \geq 0$.

Then $\mathrm{G} = (\mathrm{V}, \mathrm{E})$ *does not have Sachs graph* $\mathrm{G}^S = (\mathrm{V}^S, \mathrm{E}^S)$ *for* $\mathrm{N}^S > \min(\mathrm{N}, \mathrm{N} - \mathrm{m} + \mathrm{n})$, *where* N^S *is the number of vertices in Sachs graph* $\mathrm{G}^S = (\mathrm{V}^S, \mathrm{E}^S)$.

Proof. Suppose that G^{S} is a Sachs graph with N^{S} vertices. It is clear that $N^{\mathrm{S}} \leq N$. Let the graph G^{S} has m', n' and M vertices in sets V_1, V_2 and V_3 in order. Thus $M \leq N - m - n$ and $n' \leq n$. If a component C of G^{S} has $m'' \neq 0$ vertices in V_1 and n'' vertices in V_2 then $m'' \leq n''$, namely C can not be a loop and if $C \in C^{\mathrm{E}}(G^{\mathrm{S}})$ then $m'' = n''$. From $C \in C^{\mathrm{CY}}(G^{\mathrm{S}})$ follows that C does not have neighboring vertices from V_1, namely the neighbors of vertices from V_1 are in V_2. Thus in $C \in C^{\mathrm{CY}}(G^{\mathrm{S}})$ there is at least one vertex from V_2 between every two vertices from V_1. That is $m'' \leq n''$ and thus $m' \leq n' \leq n$.

We obtain $N^{\mathrm{S}} = M + m' + n' \leq (N - m - n) + m' + n' \leq (N - m - n) + n + n = N - m + n$. Thus $N^{\mathrm{S}} \leq \min(N, N - m + n)$. □

Remark 2. *From Lemma 2 and Theorem 1 follows that if the graph* G *of matrix* H *fulfills the properties of Theorem 1 with* $\nu = \mathrm{m} - \mathrm{n} > 0$, *then* $\epsilon = 0$ *is a* ν*-fold degenerated eigenvalue of* H. *In Ref. [6] we proved that the eigenvectors of these* $\epsilon = 0$ *eigenvalues have non-zero coefficients only on the basis vectors of set* V_1.

Definition 3. The Sachs graph G^{SR} is called reduced Sachs graph if G^{SR} is a Sachs graph that does not contain cycles with even number of vertices.

Lemma 3. *If a graph* G *has a Sachs graph* G^S *with* N^S *vertices it has also a reduced Sachs graph* G^{SR} *with* N^S *vertices*.

Proof. We obtain G^{SR} from G^{S} by replacing the cycles with even number of vertices by the non-neighboring edges of the corresponding cycles. □

Definition 4. The reduced Sachs graph G^{SR} of N^{S} vertices is a maximal reduced Sachs graph of G if for any other reduced Sachs graph $G^{\mathrm{SR}'}$ of G we have $N^{\mathrm{S}'} \leq N^{\mathrm{S}}$. Where $N^{\mathrm{S}'}$ is the number of vertices in $G^{\mathrm{SR}'}$.

Definition 5. In the graph G the chain $\mathrm{Ch}^{\mathrm{SR}}$ with odd number of vertices is called reduced chain between the vertices v_i and v_j if all the vertices of $\mathrm{Ch}^{\mathrm{SR}}$ but v_i belong to the vertices of G^{SR}, and if we walk from v_i to v_j the edges $(v_k, v_l) \in E(\mathrm{Ch}^{\mathrm{SR}})$ alternatively do not belong and belong to $C^{\mathrm{E}}(G^{\mathrm{SR}})$ (Fig. 2).

Lemma 4. *Let* Ch^{SR} *be a reduced chain between the vertices* $\mathrm{v_i}$ *and* $\mathrm{v_j}$. *Then there is such a reduced chain* $Ch^{\mathrm{SR}'}$ *between the vertices* $\mathrm{v_j}$ *and* $\mathrm{v_i}$ *that contains the same vertices as* Ch^{SR} *(Fig. 3).*

Proof. Let G^{SR} be the reduced Sachs graph that is used in the definition of $\mathrm{Ch}^{\mathrm{SR}}$. Let $G^{\mathrm{SR}'}$ be a reduced

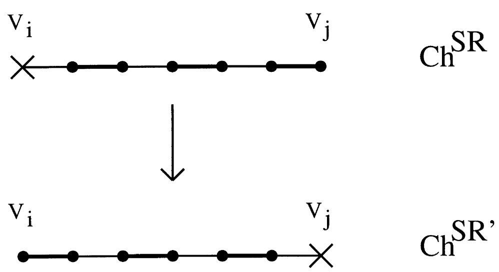

Fig. 3. A reduced chain $\mathrm{Ch}^{\mathrm{SR}}$ between the vertices v_i and v_j is transformed to a reduced chain $\mathrm{Ch}^{\mathrm{SR}'}$ between the vertices v_j and v_i. The edges of $C^{\mathrm{E}}(G^{\mathrm{SR}})$ and $C^{\mathrm{E}}(G^{\mathrm{SR}'})$ are marked by thick solid line (see Lemma 4).

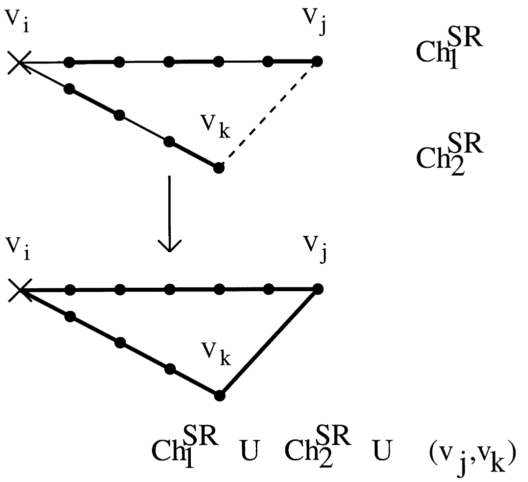

Fig. 4. A reduced chain $\mathrm{Ch}_1^{\mathrm{SR}}$ between the vertices v_i and v_j and a reduced chain $\mathrm{Ch}_2^{\mathrm{SR}}$ between the vertices v_i and v_k are transformed to the cycle $\mathrm{Ch}_1^{\mathrm{SR}} \cup \mathrm{Ch}_2^{\mathrm{SR}}(v_j,\ v_k)$ (see Lemma 5).

Sachs graph that contains the same vertices as G^{SR} but v_i is replaced by v_j, and the edges $(v_k, v_l) \in E(\mathrm{Ch}^{\mathrm{SR}}), (v_k, v_l) \in C^{\mathrm{E}}(G^{\mathrm{SR}})$ are replaced by the edges $(v_{k'}, v_{l'}) \in E(\mathrm{Ch}^{\mathrm{SR}})$ if $(v_{k'}, v_{l'}) \notin C^{\mathrm{E}}(G^{\mathrm{SR}})$. Thus the chain $\mathrm{Ch}^{\mathrm{SR}'}$ defined with the help of $G^{\mathrm{SR}'}$ is a reduced chain between the vertices v_j and v_i. □

Lemma 5. *Suppose that Ch_1^{SR} is a reduced chain*

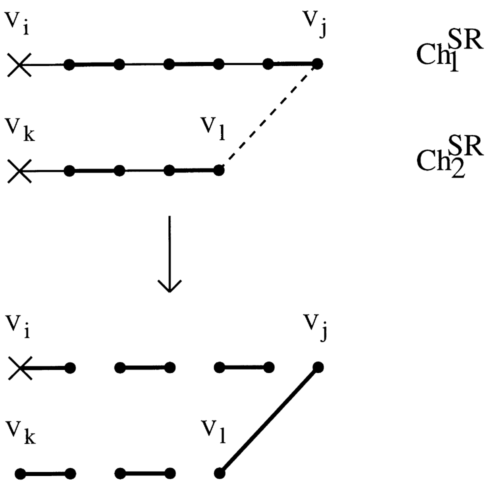

Fig. 5. A reduced chain $\mathrm{Ch}_1^{\mathrm{SR}}$ between the vertices v_i and v_j and a reduced chain $\mathrm{Ch}_2^{\mathrm{SR}}$ between the vertices v_k and v_l are transformed to the edges of reduced Sachs graph $G^{\mathrm{SR}'}$ (see Lemma 6).

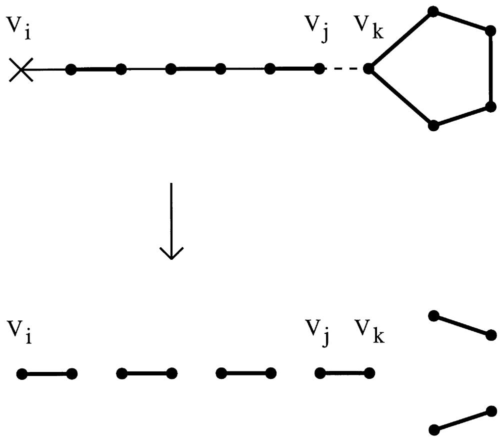

Fig. 6. A reduced chain $\mathrm{Ch}^{\mathrm{SR}}$ between the vertices v_i and v_j and a cycle G^{CY} are transformed to the edges of a reduced Sachs graph $G^{\mathrm{SR}'}$ (see Lemma 7).

between the vertices $\mathrm{v_i}$ *and* $\mathrm{v_j}$ *and Ch_2^{SR} is a reduced chain between the vertices* $\mathrm{v_i}$ *and* $\mathrm{v_k}$. *If* $(\mathrm{v_j}, \mathrm{v_k}) \in \mathrm{E(G)}$ *then there is such a reduced Sachs graph* $\mathrm{G}^{SR'}$ *of* G *that has a greater number of vertices than* G^{SR}. *The special case* $\mathrm{v_i} = \mathrm{v_k}$ *is allowed (Fig. 4).*

Proof. Let G^{SR} be the reduced Sachs graph that is used in the definition of $\mathrm{Ch}_1^{\mathrm{SR}}$ and $\mathrm{Ch}_2^{\mathrm{SR}}$. Let $G^{\mathrm{SR}'}$ be a reduced Sachs graph that contains the vertices of G^{SR} and the vertex v_i. The components of $G^{\mathrm{SR}'}$ are obtained from the components of G^{SR} by replacing the G^{E} components in $\mathrm{Ch}_1^{\mathrm{SR}}$ and $\mathrm{Ch}_2^{\mathrm{SR}}$ by the cycle of $\mathrm{Ch}_1^{\mathrm{SR}} \cup \mathrm{Ch}_2^{\mathrm{SR}} \cup (v_j, v_k)$. □

Lemma 6. *Suppose that Ch_1^{SR} is a reduced chain between the vertices* $\mathrm{v_i}$ *and* $\mathrm{v_j}$ *and Ch_2^{SR} is a reduced chain between the vertices* $\mathrm{v_k}$ *and* $\mathrm{v_l}$. *If* $(\mathrm{v_j}, \mathrm{v_l}) \in \mathrm{E(G)}$ *then there is such a reduced Sachs graph* $\mathrm{G}^{SR'}$ *of* G *that has a greater number of vertices than* G^{SR}. *The special cases* $\mathrm{v_k} = \mathrm{v_l}$ *and/or* $\mathrm{v_i} = \mathrm{v_j}$ *are also allowed (Fig. 5).*

Proof. Let G^{SR} be the reduced Sachs graph that is used in the definition of $\mathrm{Ch}_1^{\mathrm{SR}}$ and $\mathrm{Ch}_2^{\mathrm{SR}}$. Let $G^{\mathrm{SR}'}$ be a reduced Sachs graph that contains the vertices of G^{SR} and all the vertices of chain $\mathrm{Ch}_1^{\mathrm{SR}} \cup \mathrm{Ch}_2^{\mathrm{SR}}$. The components of $G^{\mathrm{SR}'}$ are obtained from the components of G^{SR} by replacing the G^{E} components in $\mathrm{Ch}_1^{\mathrm{SR}}$ and

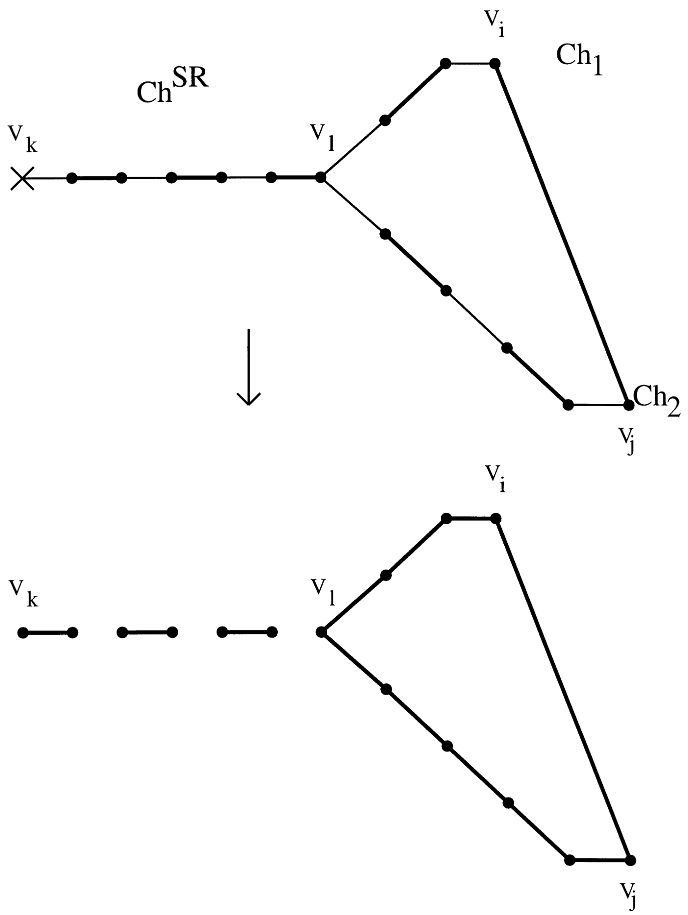

Fig. 7. A reduced chain Ch^{SR} and chains Ch_1 and Ch_2 are transformed to the cycle $Ch_1 \cup Ch_2$ and edges of $G^{SR''}$ (see Lemma 8).

Ch_2^{SR} by those edges of chain $Ch_1^{SR} \cup Ch_2^{SR}$ that are not belonging to G^{SR}. □

Lemma 7. *Suppose that Ch^{SR} is a reduced chain between the vertices v_i and v_j and there is a vertex $v_k \in V(G^{CY})$ (or $v_k \in V(G^L)$ with $(v_j, v_k) \in E(G)$, then there is such a reduced Sachs graph $G^{SR'}$ of G that has a greater number of vertices than G^{SR} (Fig. 6).*

Proof. Let G^{SR} be the reduced Sachs graph that is used in the definition of Ch^{SR} and $v_k \in V(G^{CY}$ (or $v_k \in V(G^L)$. Let $G^{SR'}$ be a reduced Sachs graph that contains the vertices of G^{SR} and the vertex v_i. The subgraph $Ch^{SR} \cup G^{CY}$ (or $Ch^{SR} \cup G^L$) is connected and have even number of vertices. The components of $G^{SR'}$are obtained from the components of G^{SR} by replacing G^{CY} (or G^E) by the corresponding edges of $Ch^{SR} \cup G^{CY}$ (or $G^{SR} \cup G^L$). □

Lemma 8. *Suppose that Ch^{SR} is a reduced chain between the vertices v_k and v_l. There are chains Ch_1 and Ch_2 between the vertices v_i, v_l and v_j, v_l, respectively. Suppose further that all the edges of Ch_1 and Ch_2 alternatively belong and not belong to $C^E(G^{SR})$ and all the vertices of Ch_1 and Ch_2 belong to the vertices of $C^E(G^{SR})$. If $(v_i, v_j) \in E(C^E(G^{SR}))$ then there is such a reduced Sachs graph $G^{SR''}$ of G that has a greater number of vertices than G^{SR} (Fig. 7).*

Proof. Let G^{SR} be the reduced Sachs graph that is used in the definition of Ch^{SR}. With the help of

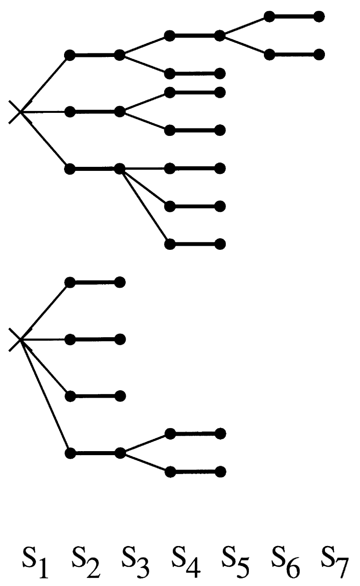

Fig. 8. A reduced forest G^{FR} with disjunct sets S_1, S_2, S_3, S_4, S_5, S_6 and S_7. The vertices of sets S_μ are on imaginary vertical lines of the figure. The edges of $E(C^E(G^{SR}))$ are marked by thick solid lines. The vertices marked by X do not belong to set $V(G^{SR})$ (see Definition 6).

Lemma 4 we can find the reduced Sachs graph $G^{SR'}$ and the reduced chain $Ch^{SR'}$ between the vertices v_l and v_k. Let $G^{SR''}$ be a reduced Sachs graph that contains the vertices of $G^{SR'}$ and the vertex v_l. The components of $G^{SR''}$ are obtained from the components of $G^{SR'}$ by replacing the C^E components of Ch_1 and Ch_2 by the cycle $Ch_1 \cup Ch_2$. The graph $G^{RS''}$ has the vertices of G^{RS} and the vertex v_k. □

Definition 6. Let G^{SR} be a maximal reduced Sachs graph of graph G and let the graphs G and G^{SR} have N and $(N-\nu)$ vertices, respectively, $(\nu > 0)$. The subgraph G^{FR} of G is called reduced forest of graph G if it fulfills the following conditions.

The vertices of G^{FR} can be partitioned into the following finite number of disjunct sets $S_1, S_2, \ldots S_\mu, \ldots$, where these sets are constructed one after the other with increasing index μ (Fig. 8).

1. $v_i \in S_1$ if and only if $v_i \notin V(G^{SR})$.
2. $v_j \in V(C^E(G^{SR}))$ for any $v_j \in S_\mu (\mu > 1)$.
3. Suppose that all the sets $S_\mu (\mu \le 2k+1)$ are known. Then $v_l \in S_{2k+2}$ if and only if $v_l \notin S_\mu$ for $(\mu \le 2k+1)$, and there is a vertex $v_{j'} \in S_{2k+1}$ for that $(v_{j'}, v_l) \in E(G)$. (There can be several $v_{j'} \in S_{2k+1}$ for that $(v_{j'}, v_l) \in E(G)$ but there is only one vertex $v_{j''} \in S_{2k+1}$ for that $(v_{j''}, v_l) \in E(G^{FR})$. In G^{FR} the vertices $v_l \in S_{2k+2}$ have only one neighbor from set S_{2k+1}.)
4. For any vertex $v_i \in S_{2l}$ there is a vertex $v_j \in S_{2l+1}$ with the edge $(v_i, v_j) \in E(C^E(G^{SR}))$, $(v_i, v_j) \in E(G^{FR})$. In G^{SR} the vertices $v_i \in S_{2l+1}$ have only one neighbor from set S_{2l} and the vertices $v_i \in S_{2l}$ have only two neighbors in G^{FR}, one neighbor from set S_{2l-1} and one neighbor from set S_{2l+1}.

Lemma 9. *Let* G^{FR} *be a reduced forest then it does not contain cycles.*

Proof. Suppose G^{FR} has a cycle CY. Then there is a vertex $v_i \in V(\mathrm{CY}), v_i \in S_\nu$ that for any other vertex $v_j \in V(\mathrm{CY}), v_j \in S_{\nu'}$ we have $\nu' \le \nu$. But from Definition 6 (points (3) and (4)) follows that $\nu' < \nu$ and any vertex $v_i \in S_\nu$ has only one neighbor $v_j \in S_{\nu'}$ in G^{FR} if $\nu' < \nu$. Thus $v_i \notin V(\mathrm{CY})$ and the reduced forest G^{FR} does not contains cycles. □

Lemma 10. *Let* G^{FR} *be a reduced forest of* G *then for* $k > 1$ *the sets* S_{2k} *and* S_{2k+1} *have the same number of vertices.*

Proof. For $v_i \in S_{2k}, (v_i, v_j) \in E(C^E(G^{SR})), v_j \in S_{2k+1}$ the edges $(v_i, v_j) \in E(C^E(G^{SR}))$ induce a one-to-one correspondence between the sets S_{2k} and S_{2k+1}. See point (4) of Definition 6. □

Lemma 11. *Let* G^{FR} *be a reduced forest of* G *and* $v_i \in S_{2k+1}, v_j \in S_{2l+1}$ *(including the case* $v_i = v_j$*) then* $(v_i, v_j) \notin E(G)$.

Proof. Let G^{SR} be the maximal reduced Sachs graph that is used in the definition of G^{FR}. Suppose that $v_i \in S_{2k+1}, v_j \in S_{2l+1}$ and $(v_i, v_j) \in E(G)$ with $v_i \ne v_j$. From Lemma 9 follows the existence of reduced chains Ch_1^{SR} and Ch_2^{SR}, where Ch_1^{SR} is a reduced chain between the vertices $v_{i'} \in S_1, v_i \in S_{2k+1}$ and Ch_2^{SR} is a reduced chain between the vertices $v_{j'} \in S_1, v_j \in S_{2l+1}$. Then if the reduced chains Ch_1^{SR} and Ch_2^{SR} are disjunct, from Lemma 6 follows that G^{SR} is not a maximal reduced Sachs graph. If the reduced chains Ch_1^{SR} and Ch_2^{SR} are not disjunct, the Lemma 4 for the common part of Ch_1^{SR} and Ch_2^{SR} gives with Lemmas 5 and 7 that G^{SR} is not a maximal reduced Sachs graph. Thus $(v_i, v_j) \notin E(G)$ for $v_i \in S_{2k+1}, v_j \in S_{2l+1}$. If $v_i = v_j$ Lemma 4 and the loop case of Lemma 7 give that G^{SR} is not a maximal reduced Sachs graph. Thus $(v_i, v_i) \notin E(G)$ if $v_i \in S_{2k+1}$. □

Lemma 12. *If* G^{SR} *is a maximal reduce Sachs graph of graph* G *and* $N^S < N$, *where* N^S *and* N *are the number of vertices in* G^{SR} *and* G, *respectively, then* G *has a reduced forest* G^{FR}.

Proof. Let us construct the sets S_μ of Definition 6 with increasing μ. As $N^S < N$ the set S_1 is not empty. If all the sets $S_\mu (\mu \le 2k+1)$ and the corresponding edges of G^{FR} are known we can construct the set S_{2k+2} as given in point (3) of Definition 6. If S_{2k+2} is the empty set then G^{FR} is already constructed. Suppose $v_i \in S_{2k+2}$ but $v_i \notin V(C^E(G^{SR}))$ in this case from Lemma 7 follows that G^{SR} is not a maximal reduced Sachs graph. Suppose $v_i \in S_{2k+2}, v_j \in S_{2k+2}$ and $(v_i, v_j) \in E(C^E(G^{SR}))$. Now follows that G^{SR} is not a maximal reduced Sachs graph. Namely in this case there are two reduced chains Ch_1^{SR} (for $v_k \in S_1$ and v_i) and Ch_2^{SR} (for $v_l \in S_1$ and v_i). There are three cases:

1. If the chains Ch_1^{SR} and Ch_1^{SR} are disjunct, there is a chain $Ch_1^{SR} \cup Ch_2^{SR}$ of even number of vertices between the v_k and v_l. Thus G^{SR} can not be maximal reduced Sachs graph.
2. If the chains Ch_1^{SR} and Ch_1^{SR} has only one common vertex there is a cycle $Ch_1^{SR} \cup Ch_2^{SR}$ in G and G^{SR} can not be maximal reduced Sachs graph.
3. If the chains Ch_1^{SR} and Ch_1^{SR} has more than one common vertices, from Lemma 8 follows that G^{SR} is not a maximal reduced Sachs graph.

Thus the points (2) and (4) of Definition 6 can also be fulfilled, and G has a reduced forest G^{FR}. □

Theorem 2. *Let* G^{SR} *be a maximal reduced Sachs graph of graph* $G = (V, E)$. *If the number of vertices in* G^S *is* $N^S = (N - \nu) < N$, *then the vertices of* G *can be partitioned into the following three disjunct sets* V_1, V_2 *and* V_3:

1. *Set* V_1: *If* $v_i \in V_1$ *and* $v_j \in V_1$ *then* $(v_i, v_j) \notin E$. *Loops are not allowed in* V_1 *and the number of vertices in set* V_1 *is* $m > 0$.
2. *Set* V_2: *If* $v_{i'} \in V_2$ *then there is at least one edge* $(v_{i'}, v_{j'}) \in E$ *with vertex* $v_{j'} \in V_1$. *The number of vertices in set* V_2 *is* $n \ge 0$.
3. *Set* V_3: $v_k \in V_3$ *if* $v_k \notin V_1$ *and* $v_k \notin V_2$.
4. $\nu = m - n$.

Proof. From Lemma 12 follows that G has a reduced forest G^{FR}. Define the following sets: $V_1 = \cup S_{2\mu+1}$ of m vertices, $V_2 = \cup S_{2\mu}$ of n vertices and V_3 contains the vertices that are not belonging to the reduced forest G^{FR}. The disjunct sets V_1, V_2 and V_3 fulfill the conditions of the Theorem. Namely:

1. From Lemmas 11 and 7 follows point (1) of Theorem 2.
2. From point (3) of Definition 6 follows point (2) of Theorem 2.
3. Point (3) of Theorem 2 is true because $v_k \in V_3$ if $v_k \notin S_{2\nu+1}$ and $v_k \notin S_{2\nu}$.
4. From point (1) of Definition 6 follows that S_1 has ν vertices and from Lemma 10 we obtain that $\nu = m - n$. □

4. Conclusions

In Theorem 1 we presented a special graph of N vertices that does not have Sachs graphs with $N, (N-1), \ldots, (N-m+n+1)$ vertices if $m > n$. Theorem 2 shows that this "special" graph structure corresponds to the general case. That is if a graph of N vertices does not have Sachs graphs with $N, (N-1), \ldots, (N-\nu+1)$ vertices it has the structure of graph of Theorem 1 for $\nu = m - n$. In practical cases it is much more easier to prove the existence of a graph structure than to prove the non-existence of Sachs graphs.

Suppose that the electronic structure of a system is described by the symmetrical square matrix $H = [H_{ij}]$ of size $N \times N$ and the graph of the shifted Hamiltonian $H' = H - H_{kk} I$ fulfills the conditions of Theorem 1 with $m - n = \nu > 0$, then $\epsilon = H_{kk}$ is at least a ν-fold degenerated eigenvalue of the Hamiltonian H and from Remark 1 follows that these eigenvectors are localized on the set V_1. We call these energy levels topologically determined energy levels because they do not depend on the actual values of the non-zero off-diagonal and $H_{ii} \ne H_{kk}$ diagonal matrix elements.

Thus the results of the previous paragraphs can be summarized without reference to graph theory in the following way.

Theorem 3. *Suppose that the* N *basis functions of the symmetrical Hamiltonian*

$$H = \sum_{i,j=1}^{N} |i\rangle H_{ij} \langle j|, \tag{5}$$

can be partitioned into three disjunct sets V_1, V_2 *and* V_3 *with the following properties:*

1. *Set* V_1: *If* $\langle i| \in V_1$ *and* $\langle j| \in V_1$ *then* $H_{ij} = H_{ji} = 0$ *and* $H_{ii} = H_{jj} = \alpha$, *where* α *is the same value for each basis functions of set* V_1. *The number of basis functions in set* V_1 *is* $m > 0$.
2. *Set* V_2: *If* $\langle i'| \in V_2$ *then there is at least one* $\langle j'| \in V_1$ *for that* $H_{i'j'} = H_{j'i'} \neq 0$. *The number of basis functions in set* V_2 *is* $n \geq 0$.
3. *Set* V_3: $\langle k| \in V_3$ *if* $\langle k| \notin V_1$ *and* $\langle k| \notin V_2$.

Thus if we can construct the above defined sets V_1, V_2 *and* V_3 *with* $m > n$ *then the value* $\epsilon = \alpha$ *is an eigenvalue of the Hamiltonian matrix* H *and this eigenvalue is at least* $(m - n)$*-fold degenerated. These eigenvalues are localized on the basis functions of set* V_1.

If the graph of the Hamiltonian *H* (Eq. (5)) does not have Sachs graph, there is an above-mentioned partition of the basis functions.

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