Topologically determined electronic energy levels and matching problems *

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Abstract

It was demonstrated previously that the topological arrangement of atoms can guarantee the existence of stable electronic energy levels. These levels are stable in the presence of off-diagonal disorder of the Hamiltonian matrix (usually of the tight-binding Hamiltonian matrix). These topologically determined energy levels were described with the help of graph theory in the framework of the existence and non-existence of Sachs-graphs. Special graph structure was suggested in order to describe the non-existence of Sachs-graphs. In the present paper it is shown that the problem of topologically determined energy levels can be studied with the help of matching theory as well.

1 Introduction

There are Hamiltonian matrices which have such kind of eigenvalues that do not depend on the actual values of the off-diagonal non-zero matrix elements. They are called topologically determined electronic energy levels as they are determined only by the appropriate distribution of the off diagonal zero matrix elements and their actual value is equal to some diagonal matrix element.

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In a previous paper [1] we presented the following theorem concerning these energy levels.

Theorem [1]. Suppose that the N basis functions of the symmetrical Hamiltonian

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

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: V_2 contains all the $\langle i|$ basis functions for which there is at least one $\langle j| \in V_1$ with $H_{ij} = H_{ji} \neq 0$. The number of basis functions in set V_2 is $n \geq 0$.
3. Set V_3: $\langle i| \in V_3$ if $\langle i| \notin V_1$ and $\langle i| \notin V_2$.
Thus if we can construct the above defined sets V_1, V_2 and V_3 with $m > n$ then the value $\varepsilon = \alpha$ is an eigenvalue of the Hamiltonian matrix H and this eigenvalue is at least $(m-n)$-fold degenerated. These eigenvalues are called topologically determined levels and the corresponding eigenfunctions are localized on the basis functions of set V_1.

We used graph theoretical methods in the demonstration of this theorem. [1, 4, 5, 6, 7, 8, 9]. The sufficient and necessary conditions of topologically determined electronic energy levels were described with the help of the existence and non-existence of Sachs-graphs [2, 3]. A Sachs-graph contains only cycle, edge and/or loop components.

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. Thus we have presented a special graph structure that is the complement of the Sachs-graph. An undirected simple graph with possible loops either has a Sachs-graph or the set of vertices can be partitioned into three disjoint sets V_1, V_2 and V_3 in the following way. Set V_1 contains only independent loop-free vertices, in set V_2 are all the neighbours of set V_1 and V_2 has more vertices than V_1. The other vertices of the graph are in set V_3. Later we shall call by $|V|$ the number of vertices in V and by $\Gamma(V)$ the neighbouring vertices of V.

In the present paper it will be shown that the topologically determined electronic energy levels can be described with the help of the matching theory [10] as well, where the existence of a perfect 2-matching in a graph G means that it contains a system of vertex-disjoint cycles and edges, that is a Sachs-graph. The other name of perfect 2-matching is q-factor [10].

Hamiltonian matrices, graphs and matchings

The characteristic polynomial of the Hamiltonian matrix of Eq. (1.) can be written as

$$D(\varepsilon) = det|\varepsilon I - H| = \sum_{n=0}^{N} a_n \varepsilon^{N-n}. \qquad (2)$$

Here I is the unit matrix and the coefficients

$$a_n = (-1)^n \sum_{\binom{N}{n}} H(i_1 i_2 ... i_n) \qquad (3)$$

are calculated with the help of the determinants $H(i_1 i_2 ... i_n)$, where we have

$$H(i_1 i_2 ... i_n) = \sum_p (-1)^{t(p)} H_{i_1 j_1} H_{i_2 j_2} ... H_{i_n j_n} \qquad (4)$$

and $t(p)$ is the parity of the p permutation $j_1 j_2 ... j_n$ of numbers $i_1 i_2 ... i_n$. In Eq. (3) the summation runs over all the principal minors of order n.

The graph $G = (V, E)$ is defined as the graph of square matrix $H = [H_{ij}]$ of size NxN if $V = \{v_1, v_2, ..., v_N\}$ is the set of N vertices and $(v_i, v_j) \in E$ if and only if $H_{ij} = H_{ji} \neq 0$. 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. Each $H_{i_1 j_1} H_{i_2 j_2} ... H_{i_n j_n} \neq 0$. product of Eq. (4) determines a Sachs-graph of $G = (V, E)$ with n vertices i_1, i_2, ... i_n and n edges (v_{i_1}, v_{j_1}), (v_{i_2}, v_{j_2}), ... (v_{i_n}, v_{j_n}). From Eq. (3) and Eq. (4) follows that $a_n = 0$ if G does not contain Sachs-graph with n vertices and we say that $a_n = 0$ accidentally if the sum in Eq. (3) contains non-zero terms. If there are no Sachs-graphs with N, $N-1$, ... $N-\nu+1$ vertices in G than from Eq. (2) follows that

$$a_N = a_{N-1} = a_{N-2} = ... = a_{N-\nu+1} = 0, \qquad (5)$$

and $\varepsilon = 0$ is a ν-fold degenerated eigenvalue of H. Here we remark that the study of $\varepsilon = \alpha = H_{kk}$ eigenvalue can be carried out with the study of the $\varepsilon = 0$ eigenvalue of the matrix $H' = H - \alpha I$.

Let G' be the graph of H'. In [1, 9] it was shown that $\varepsilon = \alpha = H_{kk}$ is a ν -fold not accidentally degenerated eigenvalue of H if and only if the vertices of graph G' can be partitioned into three disjoint sets V_1, V_2 and V_3 with the following properties. Set V_1 contains $|V_1|$ independent loop-free vertices, $V_2 = \Gamma(V_1)$, that is in V_2 are all the neighbours of V_1 and $\nu = |V_2| - |V_1| > 0$. In V_3 are the other vertices of G'. This partition of vertices is a necessary and sufficient condition for the non-existence of Sachs-graphs [1].

Now let us turn to the problem of matching and let G be an undirected simple graph. Multiple edges and loops are not allowed and we follow the definitions of ref. [10]. A set of edges in a graph G is called matching if no two edges have a vertex in common. The size of any largest matching in G is called the matching number of G and is denoted by $\nu(G)$. A 2-matching of a graph G is an assignment of weights 0, 1 or 2 to the edges of G such that the sum of weights of edges incident with any given vertex is at most 2. The size of a 2-matching is the sum of weights and the maximum size is denoted by $\nu_2(G)$. A 2-matching is called perfect if the sum of weights of edges incident with any vertex is exactly 2. It can be seen that in a perfect 2-matching the edges of weight 1 and 2 compose a system of vertex-disjoint cycles and edges which cover all vertices of graph G [10].

A perfect 2-matching of graph G is the same subgraph that we called previously Sachs-graph, and it was called q-factor by Tutte [11], who proved the following theorem which is presented also by Lovász and Plummer in Corollary 6.1.5. of [10].

Theorem (Tutte [11, 10]). A graph G has a perfect 2-matching (i. e. a q-factor) if and only if $|\Gamma(A)| \geq |A|$ for every independent set A of vertices.

Tutte's Theorem is in agreement with our statement about the existence and non-existence of Sachs-graphs. We said above namely that a graph G has a Sachs-graph (2-matching) or its vertices can be partitioned into the disjoint sets V_1, V_2 and V_3 where for the independent set of loop-free vertices V_1 we have the relation $|\Gamma(V_1)| = |V_2| < |V_1|$. The perfect agreement holds only if we do not allow loops in G as it is usually supposed in matching theory [10]. There is, however, no contradiction between the two phrasing even if there are loops in graph G of a Hamiltonian matrix H. At this time in the definition of 2-matching the weight of a loop must be taken twice and Tutte's Theorem rest valid if we replace the words "... independent set A of vertices." by "... independent set A of loop-free vertices."

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