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SELECTED TOPICS ON APPLICATIONS OF GRAPH SPECTRA

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PREFACE

The volume 13(21) of the *Collection of Papers* (*Zbornik radova*) with the title *Applications of Graph Spectra* appeared in 2009 and was soon out of print. We proposed to the Mathematical Institute of the Serbian Academy of Sciences and Arts to publish a second edition, but the Editorial Board decided to publish a new volume on the same subject with a similar title and with the same guest editors. We have chosen the title **Selected Topics on Applications of Graph Spectra** for the new volume.

The purpose of this volume and of the previous volume is to draw the attention of the mathematical community to the rapidly growing applications of the theory of graph spectra. Besides classical and well documented applications to Chemistry and Physics, we are witnesses of the appearance of graph eigenvalues in Computer Science in various investigations. There are also applications in several other fields like Biology, Geography, Economics, and Social Sciences.

A part of the Preface to volume 13(21) is reproduced below.

The new volume contains improved, modified, and extended versions of all chapters from volume 13(21) as well as the following two new chapters:

Spectral Techniques in Complex Networks (S. Gago),
Applications of Graph Spectra in Quantum Physics (D. Stevanović).

The old chapters have been technically improved including the correction of noticed typos and other mistakes. In addition the following changes have been made.

Applications of Graph Spectra: An Introduction to the Literature (D. Cvetković). Some new references have been added and the presentation of some parts is improved.

Multiprocessor Interconnection Networks (D. Cvetković, T. Davidović). New proofs of main theorems are given and the data for some interesting multiprocessor interconnection networks are better presented.

Hyperenergetic and Hypoenergetic Graphs (I. Gutman). This is a new text, with a slight overlap to the chapter *Selected Topics from the Theory of Graph Energy: Hypoenergetic Graphs*, (S. Majstorović, A. Klobučar, I. Gutman), that appeared in volume 13(21).

Nullity Of Graphs: An Updated Survey (I. Gutman, B. Borovićanin). The chapter *Nullity of Graphs*, (I. Gutman, B. Borovićanin), is extended by surveying a number of recently published results, and by updating the bibliography.

The Estrada Index: An Updated Survey (I. Gutman, H. Deng, S. Radenković). The chapter *The Estrada Index*, (H. Deng, S. Radenković, I. Gutman), is extended by surveying a number of recently published results, and by updating the bibliography.

For some more information on these Chapters see Preface to volume 13(21).

The new chapter by S. Gago is about networks with a great number of vertices called *complex networks*. Most physical, biological, chemical, technological, and social systems have a network structure. Examples of complex networks range

from cell biology to epidemiology or to the Internet. The rich information about the topological structure and diffusion processes can be extracted from the spectral analysis of the corresponding networks.

The new chapter by D. Stevanović explains that graph spectra are closely related to many applications in quantum physics: a network of quantum particles with fixed couplings can be modelled by an underlying graph, the Hamiltonian of such system can be approximated either by the adjacency or the Laplacian matrix of that graph, and then quite a few problems can be posed in terms of the eigenvalues of the graph. One particular problem of interest to quantum physicists is addressed: the existence of *perfect state transfer in networks of spin* $-1/2$ *particles*.

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Belgrade and Kragujevac, 2010

Guest Editors:
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FROM PREFACE TO VOLUME 13(21)

The purpose of this volume is to draw the attention of mathematical community to rapidly growing applications of the theory of graph spectra. Besides classical and well documented applications to Chemistry and Physics, we are witnesses of the appearance of graph eigenvalues in Computer Science in various investigations. There are also applications in several other fields like Biology, Geography, Economics and Social Sciences. A monograph with a comprehensive treatment of applications of graphs spectra is missing at the present.

The present book contains five chapters: an introductory chapter with a survey of applications by representative examples and four case studies (one in Computer Science and three in Chemistry).

We quote particular chapters and indicate their contents.

Applications of Graph Spectra: An Introduction to the Literature (D. Cvetković). This introductory text provides an introduction to the theory of graph spectra and a short survey of applications of graph spectra. There are four sections: 1. Basic notions, 2. Some results, 3. A survey of applications, 4. Selected bibliographies on applications of the theory of graph spectra.

Multiprocessor Interconnection Networks (D. Cvetković, T. Davidović). Well-suited multiprocessor interconnection networks are described in terms of the graph invariant called tightness which is defined as the product of the number of distinct eigenvalues and maximum vertex degree. Load balancing problem is presented.

Selected Topics from the Theory of Graph Energy: Hypoenergetic Graphs (S. Majstorović, A. Klobučar, I. Gutman). The energy E of a graph G is the sum of the absolute values of the eigenvvalues of G. The motivation for the introduction of this invariant comes from Chemistry, where results on E were obtained already in the 1940's. The chemical background of graph energy is outlined in due detail. Then some fundamental results on E are given.

A graph G with n vertices is said to be "hypoenergetic" if $E(G) < n$. In the main part of the chapter results on graph energy, pertaining to the inequalities $E(G) < n$ and $E(G) \geq n$ are presented. Most of these were obtained in the last few years.

Nullity of Graphs (B. Borovićanin, I. Gutman). The nullity η of a graph G is the multiplicity of the number zero in the spectrum of G. In the 1970s the nullity of graphs was much studied in Chemistry, because for certain types of molecules, $\eta = 0$ is a necessary condition for chemical stability. The chemical background of this result is explained in a way understandable to mathematicians. Then the main early results on nullity are outlined.

In the last 5–10 years there is an increased interest to nullity in mathematics, and some 10 papers on this topic appeared in the mathematical literature. All these results are outlined too.

The Estrada Index (H. Deng, S. Radenković, I. Gutman). If λ_i, $i = 1, 2, \ldots, n$, are the eigenvalues of the graph G, then the Estrada index EE of G is the sum of

the terms $\exp(\lambda_i)$. This graph invariant appeared for the first time in year 2000, in a paper by Ernesto Estrada, dealing with the folding of protein molecules. Since then a remarkable number of other chemical and non-chemical applications of EE were communicated.

The mathematical studies of the Estrada index started only a few years ago. Until now a number of lower and upper bounds were obtained, and the problem of extremal EE for trees solved. Also, a number of approximations and correlations for EE were put forward, valid for chemically interesting molecular graphs.

All relevant results on the Estrada index are presented in the chapter.

Manuscripts have been submitted in January 2009 and revised in April 2009.

Belgrade and Kragujevac, 2009

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