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Introduction to Quantum Graphs

To our families and our teachers

Preface

In this book, the name "quantum graph" refers to a graph considered as a one-dimensional simplicial complex and equipped with a differential operator ("Hamiltonian"). Works that currently would be classified as discussing quantum graphs have been appearing since at least the 1930s in various areas of chemistry, physics, and mathematics. However, as a coherent and actively pursued topic, the area of quantum graphs has experienced an explosive growth only in the last couple of decades. There are manifold reasons for this surge. Quantum graphs arise naturally as simplified models in mathematics, physics, chemistry, and engineering when one considers propagation of waves of various nature through a quasi-one-dimensional (e.g., "meso-" or "nano-scale") system that looks like a thin neighborhood of a graph. One can mention in particular the free-electron theory of conjugated molecules, quantum wires, photonic crystals, carbon nano-structures, thin waveguides, some problems of dynamical systems, system theory and number theory, and many other applications that have led independently to quantum graph models. Quantum graphs also play a role of simplified, although still non-trivial, models for studying difficult issues, for instance, Anderson localization and quantum chaos.

There are fruitful relations of quantum graphs with the older spectral theory of "standard" (combinatorial) graphs [**191**, **195**, **213**–**215**, **415**] and with what is sometimes called discrete geometric analysis [**682**]. Quantum graphs present new non-trivial mathematical challenges, which makes them dear to a mathematician's heart. As the reader will see, work on quantum graph theory and applications has brought together tools and intuition coming from graph theory, combinatorics, mathematical physics, PDEs, and spectral theory.

In the new millennium, these relations between the various topics leading to quantum graphs were noticed, which has triggered a series of interdisciplinary meetings and intensive communication and cooperation among researchers coming from different areas of science and engineering. Surveys and collections of papers on quantum graphs and related issues have started to appear (e.g., [**98**, **121**, **122**, **126**, **161**, **353**,

421, 438, 477–480, 536, 614, 615, 622]). These surveys, however, usually focus on special features of quantum graph theory and there is still no comprehensive introduction to the topic, which is why the authors decided to write this text. The book is intended to serve a dual purpose: to provide an introduction to and survey of the current state of quantum graph theory, as well as to serve as a reference text, where the main notions and techniques are collected.

The authors are indebted to many colleagues, from whom they have learned over the years a great deal about quantum graph theory and related issues. This includes, in particular, M. Aizenman, R. Band, J. Bolte, R. Carlson, Y. Colin de Verdiere, P. Exner, A. Figotin, M. Freidlin, L. Friedlander, S. Fulling, S. Gnutzmann, R. Grigorchuk, J.M. Harrison, J. P. Keating, E. Korotyaev, V. Kostrykin, M. Kotani, T. Kottos, L. Kunyansky, S. Molchanov, V. Nekrashevich, S. Novikov, K. Pankrashkin, B. Pavlov, O. Post, H. Schantz, R. Schrader, M. Shubin, U. Smilansky, A. Sobolev, M. Solomyak, T. Sunada, A. Teplyaev, B. Vainberg, I. Veselić, and B. Winn. The second author has been significantly influenced by the late M. Birman, R. Brooks, and V. Geyler. We cordially thank S. Fulling, W. Justice and our graduate students N. Do, W. Liu and T. Weyand for their critical reading of the manuscript and numerous corrections.

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Finally, we are grateful to our families for their limitless patience.

Gregory Berkolaiko and Peter Kuchment
College Station, TX
July 2012

Introduction

In this book, our goal is to introduce the main notions, structures, and techniques used in quantum graph studies, as well as to provide a brief survey of more special topics and applications. This task has shaped the book as follows: we present in detail the basic constructions and frequently used technical results in Chapters 1 and 2, devoted to quantum graph operators, and Chapters 3 – 5, which address various issues of the spectral theory of quantum graphs. The remaining two chapters are of review nature and thus less detailed; in most cases the reader will be directed to the cited literature for precise formulations and proofs. Using graphs as models for quantum chaos is considered in Chapter 6. Chapter 7 provides a brief survey of various generalizations and applications. The reader will notice that the area is developing very fast; had we tried to be more specific in this chapter, it would be outdated by the time of publications anyway.

Our intent was to make the book accessible to graduate and advanced undergraduate students in mathematics, physics, and engineering.

Since a variety of techniques are used, for the benefit of the reader we introduce the main notions and relevant results in graph theory, functional analysis, and operator theory in a series of Appendices.

In order to make reading smoother, we normally do not include references in the main text of the chapters, collecting them, as well as additional comments, in the specially devoted last section of each chapter. We also have not tried to make the considerations too general. For instance, we mostly treat the second derivative operators on quantum graphs, while considerations could be easily extended to the more general Schrödinger operators. When we do mention more general operators, we do not look for the most general conditions on the coefficients (potentials), settling for some reasonable conditions that make the techniques work.

Contents

CHAPTER 1

Operators on Graphs. Quantum graphs

In this chapter, we introduce the main players of the quantum graph theory: metric graphs and differential operators on them. A graph consists of a set of points (vertices) and a set of segments (edges) connecting some of the vertices (Fig. 1).

More notions and results concerning graph theory can be found in Section 1.1) and Appendix A. Most mathematicians are already familiar with combinatorial graphs (which we survey briefly in Section 1.1), where the vertices are the main players and the edges merely indicate some relations between them. In a metric graph, in contrast, attention is focused on the edges. Metric graphs are introduced in Section 1.3. Quantum graphs are essentially metric graphs equipped with differential operators. Such operators (Hamiltonians) are considered in Section 1.4. The main operator under consideration acts as the second derivative along the edges with "appropriate" conditions at junctions (vertices). These conditions generalize the boundary conditions for ODEs. Here, a lot of attention is devoted to describing what are the "appropriate" conditions. Considering the quantum graph from the point of view of waves propagating along edges and scattering at vertices and other more advanced (but fundamental) topics are deferred to Chapter 2.

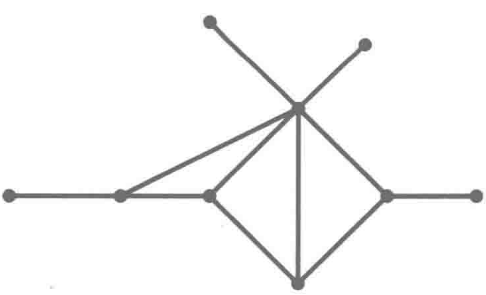

FIGURE 1. A graph

1.1. Main graph notions and notation

We start by introducing some common graph notions and notation used throughout the text. The reader is also referred to Appendix A for these and some other notions from the graph theory.

A **graph** Γ consists of a finite or countably infinite set of vertices $\mathcal{V} = \{v_i\}$ and a set $\mathcal{E} = \{e_j\}$ of edges connecting the vertices. The edges are undirected. As we will see in Section 1.4, in the quantum graph situation one can usually assume absence of loops and multiple edges, since if these are present, one can break them into pieces by introducing new intermediate vertices. We thus will be assuming mostly that loops and multiple edges between vertices are not present. We will use the notation $E := |\mathcal{E}|$ and $V := |\mathcal{V}|$ for the number of edges and vertices correspondingly. The notation $v \in e$ will be taken to mean that v is a vertex of the edge e. Two vertices u and v will be called **adjacent** (denoted $u \sim v$) if there exists an edge connecting them. A graph Γ is fully specified by its $|\mathcal{V}| \times |\mathcal{V}|$ **adjacency matrix** A_Γ. In the simplest case when there are no loops or multiple edges, the elements of the adjacency matrix are given by

$$A_{u,v} = \begin{cases} 1 & \text{if } u \sim v, \\ 0 & \text{otherwise.} \end{cases} \tag{1.1.1}$$

More generally,

$$A_{u,v} = \left|\{e \in \mathcal{E} : u \in e, v \in e\}\right|. \tag{1.1.2}$$

The **degree** d_u of a vertex u is the number of edges emanating from it, $d_u = \sum_{v \in \mathcal{V}} A_{u,v}$. All degrees are assumed to be finite (**local finiteness** of the graph).

We will denote by D_Γ the **degree matrix**, i.e. the diagonal $|\mathcal{V}| \times |\mathcal{V}|$ matrix with the diagonal entries d_v:

$$D_{u,v} = d_v \delta_{u,v}, \tag{1.1.3}$$

where $\delta_{u,v}$ is the Kronecker delta

$$\delta_{u,v} = \begin{cases} 1 \text{ if } u = v, \\ 0 \text{ otherwise.} \end{cases}$$

Sometimes it becomes necessary to consider directed edges. A graph is called **directed graph** or **digraph**, if each of its edges is assigned a direction. In other words, each edge has one **origin** and one **terminal vertex**. Directed edges will be called **bonds**. The set of all bonds is denoted by $\mathcal{B}$. We will use the shorthand notation $B := |\mathcal{B}|$ for the total number of bonds in a directed graph Γ. The origin and terminal