Math. & Comput. Sci., 7(2) (2026), 125–136
Online: ISSN 2717-2708
Mathematics and Computational Sciences
Journal Homepage: http://mcs.qut.ac.ir/mcs

A review on quantum graphs: From mathematical foundations to applications

Kavya Mangattu Sudheer [a], Nandhini Sivasubramaniam [a,*]

[a] Department of Mathematics, School of Advanced Sciences, Vellore Institute of Technology, Vellore, India.

Abstract

Quantum graphs provide a rigorous framework for modelling quantum dynamics on network-like structures, where edges represent one-dimensional wires and vertices encode interaction conditions. Since their introduction as models for wave propagation and molecular systems, quantum graphs have grown to become an essential tool in mathematical physics, providing information on spectral, transport, and scattering phenomena. The mathematical foundations of quantum graphs are reviewed in this review, covering self-adjoint operators, metric graph formalisms, and vertex conditions that control the behaviour of wave functions. Next, we discuss important developments in spectrum theory that make quantum graphs strong models for quantum chaos and universal spectral statistics, including resonance features, eigenfunction statistics, and spectral gap optimisation. Stability analyses and inverse spectrum problems broaden the theoretical scope of the framework, while extensions to leaky, transparent, and random quantum graphs show how versatile it is. The survey emphasises the function of quantum graphs as a link between discrete and continuous models by combining these viewpoints. We conclude by describing open difficulties in the areas of spectral invariants and random graph models.

Keywords: Quantum graphs, Spectral theory, Quantum chaos, Scattering, Resonance

2020 MSC: 81Q35, 05C50

1. Introduction

Quantum graphs are mathematical models where quantum movements are constrained to one dimensional edges connected at vertices under specified boundary conditions. This framework combines the combinatorial structure of graphs with the continuous analysis of differential operators, making quantum graphs an effective bridge between discrete and continuous systems.[38, 10]

The study of quantum graphs originated in the 1930s with Paulings early models of conjugated hydrocarbons, where electrons were approximated as moving along molecular bonds represented by graph edges[46]. Since then, quantum graphs have emerged as versatile models in physics, chemistry, and engineering. They are used to describe wave propagation in thin structures, mesoscopic systems, microwave networks, and photonic crystals[26].

A central motivation for quantum graph theory is its ability to capture spectral properties of quantum systems in a tractable framework. The eigenvalue spectrum of quantum graphs provides insights into

*Corresponding author
Email addresses: kavya.ms@vit.ac.in (Kavya Mangattu Sudheer), nandhini.s@vit.ac.in (Nandhini Sivasubramaniam)
doi: 10.30511/mcs.2025.2075553.1566
Received: 23 October 2025   Accepted: 29 November 2025

resonance phenomena, transport properties, and universal spectral statistics. In particular, they serve as simplified yet exact models for studying quantum chaos, where spectral correlations of quantum systems exhibit universality described by random matrix theory[37].

From a mathematical perspective, quantum graphs are governed by differential operators such as the Laplacian or Schrödinger operator defined on the graph edges. To ensure self-adjointness, vertex boundary conditions must be imposed, leading to a rich interplay between functional analysis, operator theory, and spectral geometry[38]. The exact solvability of spectral problems on graphs has enabled progress in understanding nodal domain statistics, spectral gaps, inverse problems, and scattering theory.

Beyond pure mathematics, extensions of the quantum graph framework have been developed to include leaky graphs (where particles may tunnel into higher dimensions), transparent boundary models, and random/disordered graphs, which provide toy models for complex quantum systems exhibiting localization and universality [17, 22, 12]. These advances highlight the versatility of quantum graphs as both mathematical objects and applied physical models.

This review provides a comprehensive survey of the mathematical foundations, spectral theory, scattering phenomena, and extensions of quantum graphs. We emphasize their dual role, as rigorous mathematical models and as effective tools in applied physics. We also highlight open problems in spectral invariants, inverse spectral theory, and random graph models, pointing toward directions for future research.

2. Quantum Graph and its Mathematical Foundations

Quantum graphs are constructed as metric graphs, where each edge is assigned a length and carries a differential operator, typically the Laplacian or Schrödinger operator. Functions are defined edgewise, and their behaviour at the vertices is constrained by boundary conditions that guarantee the self-adjointness of the operator. These elements form the rigorous mathematical backbone of the theory.

2.1. *Metric Graphs and Operators*

A metric graph $\Gamma = (V, E)$ is the graph that consists of a finite set of vertices V and edges E, each edge $e \in E$ identified with an interval $[0, l_e]$ for finite edges or $[0, \infty)$ for infinite case. A quantum graph is a pair (G, H), where $G = (v, E)$ is a metric graph and $H = L^2(G)$ is the Hilbert space of square-integrable functions defined on its edges, which is equipped with an operator and appropriate vertex conditions. Each edge $e \in E$ is identified with a function $f \in L^2(G)$, where

$$f = \{f_e : e \in E, f_e \in L^2(0, l_e)\}. \tag{2.1}$$

Operators are mathematical structures that can often be self-adjoint. Usually, the operators that are used includes, Schödinger operator, Laplacian operator, Dirac operator and Pseudo-Differential operators. The key mathematical problem is to define appropriate vertex boundary conditions such that the global operator, which is the direct sum of the edgewise operators coupled with the vertex condition, is self-adjoint.

2.2. *Vertex Boundary Conditions and Self Adjointness*

Vertex conditions determine how wave functions transmission and reflects at the vertices. These conditions determine the self-adjoint extension of the operators that was considered on the edges. The most general class of self-adjoint vertex conditions was characterized by Kostrykin and Schrader[35]. For a vertex of degree d, let F be the vector $(f_1(v), f_2(v), ..., f_d(v))^t$ of the vertex values of the function along each edge, and $F' = (f_1'(v), f_2'(v), ..., f_d'(v))^t$ be the vector of the vertex values of the derivatives taken along the edges in the outgoing direction at the vertex v, then

$$A_v F + B_v F' = 0 \tag{2.2}$$

is the most general form of such conditions where $A, B \in \mathbb{C}^{d \times d}$ satisfying $AB^\dagger = BA^\dagger$ and $\text{rank}(AB) = d$.

Some of the significant cases of vertex conditions that are used:

- Kirchhoff condition: The sum of outgoing derivatives at a vertex is zero,

$$\sum_{e=1}^{d} f'_e(v) = 0. \tag{2.3}$$

- Dirichlet condition: All the indecent functions vanishes at the vertex.
- Neumann condition: All the derivatives vanish at the vertex.
- δ- type coupling: The functions are continuous across the vertex, with a jump in derivatives controlled by the real parameter α,

$$\sum_{e=1}^{d} f'_e(v) = \alpha f(v). \tag{2.4}$$

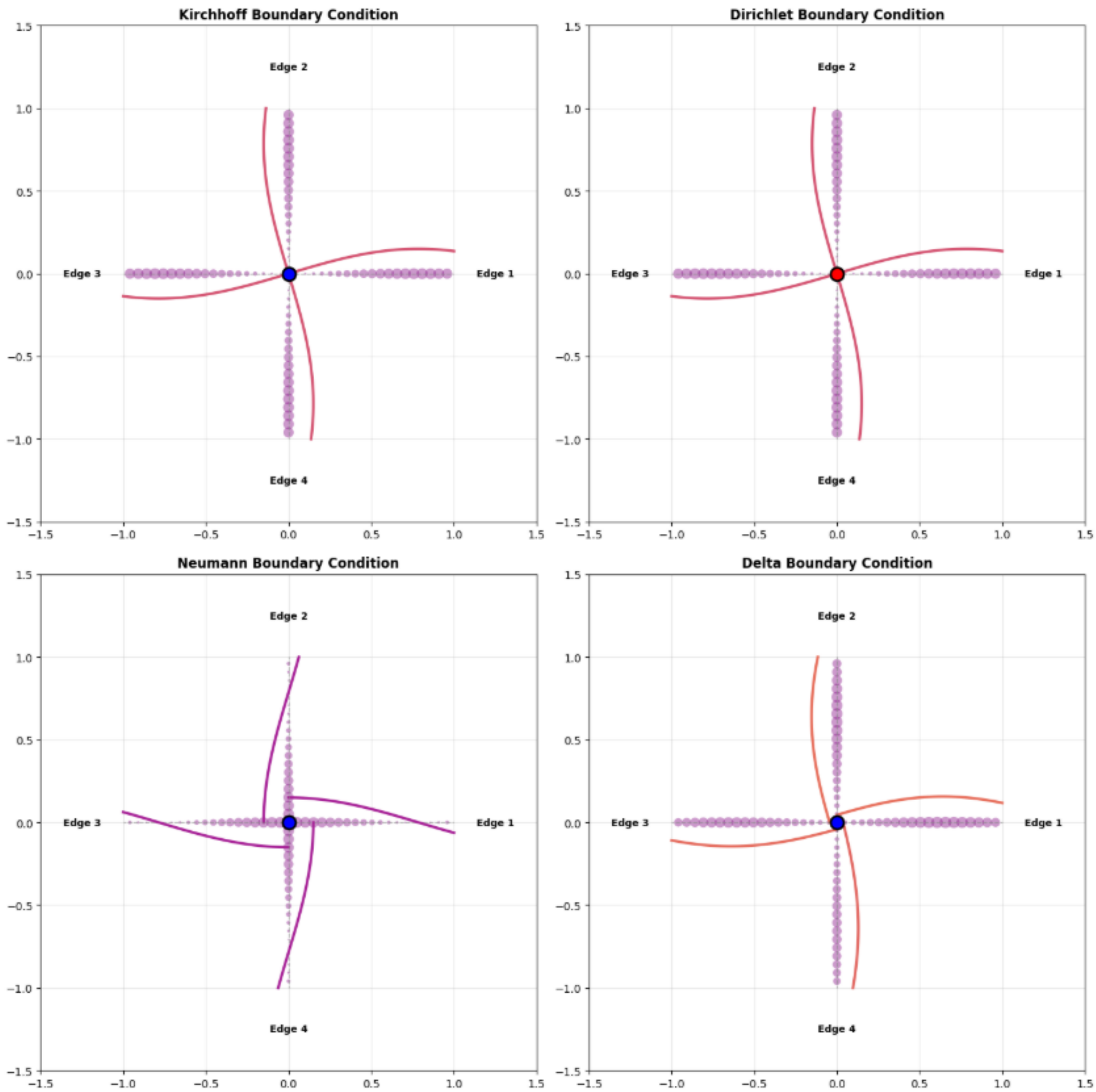

Figure 1: Wavefunction behaviour on a four-edged quantum graph under different vertex conditions.

As illustrated in Figure 1 the choice of the boundary condition changes the behaviour of the quantum graph. Oscillating coloured curves represent the real part of the wavefunction, while the purple points trace the corresponding probability density along each edge. The colour of the central vertex reflects the strength of the wave at that point, helping to see whether the wave passes smoothly through the junction, is forced to drop to zero, or is modified otherwise by the chosen boundary condition.

3. Spectral Theory and Quantum chaos

The spectral theory of quantum graphs is the study of the eigenvalues and eigenfunctions of the Hamiltonian operator H defined on a metric graph.

For finite compact graphs, the spectrum of H is real and discrete since it is self-adjoint given appropriate vertex conditions. The eigenvalue problem

$$Hf = \lambda f \tag{3.1}$$

reduces to matching eigenfunctions along edges under vertex boundary conditions. The preferred eigenvalues are determined by a secular equation, usually written in the terms of the bond scattering matrix $S(k)$:

$$\det(I - U(k)) = 0, U(k) = e^{ikL}S, \tag{3.2}$$

where $k = \sqrt{\lambda}$, L is the diagonal matrix of edge lengths, and S encodes vertex scattering. Where as the spectrum for non-compact or infinite graphs may have resonant and continuous components. Spectral theory on quantum graphs provides deep insights into the wave dynamics and statistical features of quantum states, and have been central to study of quantum chaos.

Recent work continues to deepen the connection between geometry and spectral data. Kennedy[34] presents a systematic account of the geometric spectral theory of quantum graphs, focusing on eigenvalue optimization under geometric constraints. Matsuda [43] introduced algebraic connectedness and bipartiteness for quantum graphs via homomorphisms. These advancements demonstrate that the spectral analysis of quantum graphs is an important foundation for new algebraic and geometric frameworks, along with being an aid for chaos theory. It has provided rigorous models for quantum chaos, nodal phenomena and universality in eigen statistics, making them central to modern mathematical physics[10, 26, 36].

3.1. Eigenfunction Statistics and Nodal Domains

The nodal structure of eigenfunctions provides deep connections between graph topology and spectral behaviour. Early results established Courant-type bounds on nodal domains[9], but recent work has refined this theory. Hofmann et al. extended Pleijels theorem to quantum graphs, proving that the asymptotic nodal ratio ν_n/n(nodal domains divided by eigenfunction index) has only finitely many accumulation points[30]. Plümer et al. showed that fully supported eigenfunctions obey nodal constraints distinct from those in higher-dimensional manifolds[48].

Baptista et al. recently investigated Neumann domains and spectral minimal partitions, generalizing Courant-type bounds and linking nodal partitions with optimization of spectral energies[8]. Band & Charron established a SturmHurwitz theorem on quantum graphs, bounding the number of zeros of linear combinations of eigenfunctions, a phenomenon unique to graphs compared to intervals or manifolds[7].

Furthermore, Alon et al. analysed the distribution of nodal surplus (the deviation of nodal count from a baseline expectation) and demonstrated universal statistical behaviour across large random graphs, reinforcing parallels with random matrix universality[2].

3.2. Spectral Gap Optimization

In quantum graph research, optimising spectral gaps has emerged as a key mathematical topic. Recent research has refined the findings of earlier work that proved the dependence of eigenvalues on edge lengths and boundary conditions[39].Exner analysed generalized vertex couplings and proved that among star graphs of fixed total edge length, the ground-state eigenvalue λ_1 is maximized by equilateral configurations, while higher eigenvalue bounds are realized by equilateral figure-8 graphs[19, 21].

Conversely, Campbell & Dooley presented spectral derivative techniques for graph bottleneck optimisation, employing spectral partitioning and Fiedler vectors to create rewiring plans that maximise or minimise spectral gaps[13]. These developments demonstrate the expanding relationship between applied network optimisation and spectral geometry.

3.3. Universality and Quantum Chaos

One of the most practical models for quantum chaos is a quantum graph, that exhibits characteristics like nodal universality, eigenvalue rigidity, and level repulsion. They are perfect areas for proving universality conjectures in spectral statistics, as they can support accurate trace formulas[37]. Recent developments in spectral optimization and nodal domain theory reinforce its use as a link between statistical descriptions using Random Matrix Theory and deterministic spectral geometry.

4. Resonances and Scattering Phenomena

Quantum graphs are excellent tools for investigating spectral statistics, as their energy levels can smoothly transition from integrablelike patterns to chaotic ones. Resonance poles of the scattering matrix encode transport phenomena and provide insight into localization, decay and wave interference[18].

Quantum graphs that include semi-infinite leads exhibit fundamentally different spectral behaviour compared to compact graphs. While compact graphs possess purely discrete spectra, open graphs with attached leads display continuous spectra intertwined with resonancescomplex poles encoding metastable states and decay dynamics. These phenomena connect spectral graph theory with scattering theory, providing a unifying framework for analysing transport, resonance asymptotics, and quantum chaos [38, 18].

Recent works extend this framework to include unbalanced graphs, topological bound states, and stability analyses of resonances under geometric or coupling perturbations [32, 31, 29, 25, 21]

Scattering theory on quantum graphs plays a central role in connecting their mathematical structure with physical properties such as transmission, reflection, and resonance lifetimes. This section goes over the definition of resonances using resolvent poles, the formalism of scattering matrices, and recent advances like hidden eigenvalues, entropy measures of scattering, and applications driven by quantum information.

4.1. Scattering on Quantum Graphs

A quantum graph with leads is a network where a finite core (the compact graph) is connected to semi-infinite wires, called leads.

Consider a metric graph G composed of finite internal edges and semi-infinite external leads. At each edge e, the wave function satisfies the stationary Schrödinger equation

$$-\frac{d^2 f_e}{dx^2} = k^2 f_e \tag{4.1}$$

whose general solution on each lead is a superposition of incoming and outgoing plane waves:

$$f_e(x) = a_{in,e} e^{-ikx} + a_{out,e} e^{ikx} \tag{4.2}$$

Vertex coupling conditions impose continuity of f and conservation of current at each vertex:

$$A_\nu F + B_\nu F' = 0 \tag{4.3}$$

where F and F′ denote the boundary values of functions and derivatives on all incident edges. For self-adjoint pairs (A, B), the scattering matrix $S(k)$ relates incoming and outgoing amplitudes:

$$a_{out} = S(k)a_{in} \tag{4.4}$$

When the coupling is self-adjoint, $S(k)$ is unitary for real k, ensuring flux conservation [35, 22].

Recent investigations expand this classical setting. The Impedance Statistics of Cable Networks model [25] treats the quantum graph as a random electrical network, examining how impedance fluctuations translate into scattering variability. These probabilistic analogues provide insight into disorder-induced scattering and transport fluctuations relevant to mesoscopic physics.

4.2. Resonances and Resolvent Poles

Resonances formalize quasi-bound or metastable states in open quantum graphs. Mathematically, resonances correspond to poles of the meromorphic continuation of the resolvent operator or, equivalently, of the scattering matrix $S(k)$ into the complex planes lower half:

$$k_0 = \alpha - i\beta, \quad \beta > 0 \tag{4.5}$$

This pole describes a decaying state with a lifetime proportional to β^{-1} Equivalently, resonances can be defined as eigenvalues of the Hamiltonian under purely outgoing boundary conditions. The equivalence of these definitions has been established for broad classes of graphs [22].

Recent progress clarifies the distribution and geometric sensitivity of these poles. Ingremeau [32, 31] derived lower bounds for the number of resonances in unbalanced open graphs and showed that weakly open graphs exhibit resonances exponentially close to the real axis, approximating the spectrum of the closed system. Evans and Maltsev [29] introduced topological bound stateseigenvalues not arising from the secular equation zeros but from singularities in the vertex scattering matrixrevealing deeper geometric constraints on resolvent poles.

4.3. Resonance Asymptotics and Counting Laws

The asymptotic distribution of resonances encodes both geometric and dynamical information. Analogues of Weyls law hold for quantum graphs with leads. The number $N(R)$ of resonances with $|k| < R$ satisfies

$$N(R) \sim \frac{L_{tot}}{\pi} R, \quad R \to \infty, \tag{4.6}$$

where L_{tot} is the total length of finite edges [38]. This effectively reflects the one-dimensional structure of the edges.

Refinements of this asymptotic behaviour highlight the influence of topology and coupling. For tree-like or symmetric graphs, resonance gaps (regions devoid of poles) can occur. For more complex graphs, resonances may accumulate along logarithmic spirals in the complex plane [18]. Statistical analyses of impedance spectra in disordered quantum networks further confirm the linear-growth law on average and reveal random deviations corresponding to chaotic scattering regimes [25].

4.4. Scattering Phase Shifts, Transport, and Quantum Chaos

Transport characteristics of open quantum graphs are determined by the energy dependence of the scattering matrix. The scattering phase shift

$$\Theta(k) = \arg\det S(k) \tag{4.7}$$

captures cumulative delay effects and is directly linked to the density of states via the Friedel sum rule:

$$\rho(k) = \frac{1}{2\pi}\frac{d\Theta(k)}{dk}. \tag{4.8}$$

The determinant relation

$$\det(I - U(k)) = \det(S(k))e^{-ikL_{tot}}, \tag{4.9}$$

where, $U(k)$ is the bond-scattering matrix of the closed graph, bridges the spectral theory of closed graphs and the transport properties of open ones [37]. If each matrix element $S_{ij}(k)$ represents the complex amplitude of a wave that enters through lead j and exits through lead i.

Then the corresponding transmission probability is given by:

$$T_{ij}(k) = |S_{ij}(k)|^2 \tag{4.10}$$

This quantity measures the probability that a quantum particle (or wave) incident on lead j will be transmitted to the lead i at energy $E = k^2$.

Recent work connects transport with spectral optimization. Preferred orientation vertex conditions, which break time-reversal symmetry, significantly modify transport properties and spectral gaps, offering new methods for spectral engineering in networks [13]. Statistical analyses [25] suggest that random fluctuations in coupling strengths or edge lengths lead to universal conductance fluctuations analogous to those in mesoscopic quantum systems. These phenomena provide a rigorous mathematical setting for studying quantum chaos and universality in graph-based models.

5. Stability, Inverse Problems, and Extensions of Quantum Graphs

Quantum graphs are not only a playground for spectral theory and quantum chaos, but also a fertile ground for the study of stability phenomena, inverse spectral problems, and generalized extensions such as leaky and random quantum graphs. These directions deepen the mathematical structure of the theory while opening new applications in physics and network science.

5.1. Stability of Spectral Properties

Stability analysis examines how spectral quantities such as eigenvalues, resonances, or nodal structures respond to perturbations in graph geometry, edge lengths, or coupling conditions. Early results showed that small perturbations of edge lengths lead to continuous but non-trivial changes in eigenvalues, with implications for wave localization[40]. Berkolaiko and Kuchment demonstrated that magnetic perturbations cause predictable changes in nodal counts, yielding stability bounds on nodal statistics[10].

Recent results extend stability to vertex conditions, Exner and Lipovský analysed general self-adjoint couplings at the vertices and proved stability criteria for spectral gaps under coupling perturbations[16]. Such results have direct relevance for the robustness of photonic and mesoscopic networks against structural disorder.

5.2. Inverse Problems

Inverse spectral problems ask whether the geometry or topology of a graph can be reconstructed from spectral data. The classical question Can one hear the shape of a graph? has been studied since the works of Gutkin and Smilansky (2001)[28]. While isospectral non-isomorphic graphs exist, reconstruction is possible under generic assumptions, using tools such as trace formulas and resonance asymptotics.

Recent advances include the study of inverse nodal problems. Band, Berkolaiko, and Smilansky (2020) showed that nodal counts, when combined with spectral data, can uniquely determine certain classes of graphs[1]. Avdonin and Pivovarchik (2021) extended inverse spectral methods to quantum trees, using boundary control approaches[6]. Such results show that quantum graphs are central to the general theory of inverse problems, linking PDE analysis with combinatorial geometry.

5.3. Leaky and Transparent Quantum Graphs

Traditional quantum graphs constrain wave propagation strictly along edges, but extensions to leaky graphs allow wave functions to penetrate into the embedding Euclidean space. Exner and Turek developed rigorous models of leaky quantum graphs by coupling metric graphs with two-dimensional Schrödinger operators[17]. These systems better capture realistic phenomena such as leakage in optical fibres or molecular waveguides.

Another extension involves transparent boundary conditions, which allow partial transmission of waves at vertices. Such models have been applied in the study of open quantum systems and resonance phenomena, leading to refined scattering theories[39].

5.4. Random Quantum Graphs

Randomness in edge lengths, connectivity, or vertex couplings provides a natural framework for studying localization and universality in spectral theory. Random quantum graphs exhibit phenomena reminiscent of Anderson localization, where disorder leads to exponential decay of eigenfunctions[4].

More recently, Anantharaman and Sabri analysed resonance distributions on random graphs, proving analogues of the Weyl law for disordered systems[3]. In parallel, Berkolaiko and Kuchment investigated random edge perturbations and their effect on spectral band structure, with implications for random photonic crystals[11]. Random quantum graphs thus provide a tractable model for bridging deterministic spectral geometry and probabilistic analysis.

6. Quantum Graphs as Bridges Between Discrete and Continuous Models

Quantum graphs occupy a unique position between discrete graph theory and continuous spectral geometry. Their formulation combines the combinatorial structure of a discrete network with the analytic tools of differential operators on metric spaces, providing a unifying framework that is simultaneously tractable and physically realistic. This duality has led to applications across physics, mathematics, and engineering.

6.1. DiscreteContinuous Duality

Quantum graphs extend discrete Laplacian on combinatorial graphs into the metric setting, where edges carry lengths and support differential operators. The discrete Laplacian on a finite graph with a set of vertex V and an edge set E is defined by

$$(\Delta f)(v) = \sum_{u \sim v} (f(v) - f(u)), v \in V, \tag{6.1}$$

while the quantum graph Laplacian acts as

$$(Hf)_e(x) = -\frac{d^2}{dx^2} f_e(x), x \in (0, l_e). \tag{6.2}$$

The connection is established through boundary conditions at vertices (such as Kirchhoff, Dirichlet, Robin), which reduce in certain limits to discrete Laplacian constraints[14, 39]. This duality allows the transfer of intuition and methods between combinatorial graph theory and continuous PDE analysis.

6.2. Approximation of Manifolds and Waveguides

Quantum graphs also serve as effective models for thin networks and waveguides. Asymptotic analysis shows that Schrödinger operators on thin domains converge to quantum graph Hamiltonians in the limit where the cross section shrinks to zero [20]. This provides rigorous justification for modelling nanowires, photonic crystal fibres, and molecular junctions by quantum graphs rather than full-dimensional PDEs.

Recent work by Post established convergence theorems linking Laplacians on thin manifolds to metric graph operators [49]. Extensions include random thin structures and leaky graphs embedded in $\mathbb{R}$ which account for transverse leakage effects.

6.3. Quantum Networks and Transport

From a physics perspective, quantum graphs provide natural models of quantum transport in mesoscopic systems. The scattering matrix $S(k)$, encodes how the incoming waves from the external leads scatter through the network as given in 4.4. This formulation is widely used to study conductance in nanoscale devices and photonic networks[15].

A key advantage of quantum graphs is that transport properties can often be computed explicitly, using secular equations and trace formulas, enabling comparison between deterministic and random models. Recent work in quantum transport on graph-like structures has accelerated rapidly due to applications in quantum information routing, photonic circuitry, and nanoscale device engineering. A major development in this area is the study of chiral quantum walks, where complex edge phases break time-reversal symmetry. Yu and Cai [52] showed that such phase manipulation enables highly directional transport on simple Y-junctions. Building on this, Annoni, Frigerio and Paris [5] demonstrated that similar chiral modulation on chain-like graphs can significantly enhance transport probabilities.

Alongside directional transport, quantum graphs have also become promising platforms for entanglement generation. Silva, Bazeia and Andrade [50] revealed that simple graphs can produce maximally entangled states when equipped with appropriate scattering or vertex conditions, suggesting that compact entanglement-generation devices may be realizable in experimental settings such as microwave networks.

Together, these developments show that quantum graphs are no longer purely theoretical constructs, they have become highly tunable and physically meaningful models capable of supporting advanced quantum transport, entanglement generation, and device-level functionality relevant to emerging quantum technologies.

6.4. Hybrid Models and Applications

Quantum graphs also appear in hybrid models that blend discrete and continuous dynamics:

- Quantum-classical hybrids are used in quantum chemistry to approximate molecular orbitals localized on bonds[47].
- Photonic applications are networks of coupled optical fibres that can be modelled as quantum graphs with complex potentials[44].
- Biological networks are Exciton transport in photosynthetic complexes that has been studied using quantum walk models on graphs, which are closely related to quantum graph Laplacians[45].

Such applications highlight the versatility of the framework, extending beyond purely mathematical interest to experimentally realizable systems.

7. Computational Tools for Quantum Graph Modelling

Modern research on quantum graphs increasingly relies on computational tools to explore complex boundary conditions, simulate quantum dynamics, and visualize spectral structures. One of the most sophisticated platforms currently available is QGLAB, a MATLAB package developed by Goodman, Conte, and Marzuola [27]. QGLAB provides a comprehensive numerical framework for generating metric graphs, enforcing boundary conditions, computing spectra, and solving time-dependent non-linear equations. Its robust implementation makes it a valuable tool for experimentalists and theorists working on both linear and non-linear quantum graph systems.

In the Python environment, the Quantum Lattice Boltzmann Method (QLBM) has become an important tool. Georgescu, Schalkers, and Möller [24] introduced this framework to simulate quantum dynamics across any kind of geometries, including multi-dimensional domains. Although not exclusive to metric graphs, QLBM can be adapted to graph-like domains and discrete models, making it a suitable platform to simulate transport, scattering, and localization phenomena across complex networks.

The use of graphs in quantum research has been further developed by various computing frameworks. Libraries such as GraphiQ enable the construction and manipulation of photonic graph states, emphasizing the connection between graph structures and quantum information encoding. Additionally, emerging tools like the Quantum Evolution Kernel (QEK) apply graph-based quantum dynamics to machine learning tasks, representing a novel intersection between quantum graph theory and data-driven applications.

8. Open Problems and Future Directions

Quantum graph theory has matured into a well-developed framework at the intersection of spectral analysis, graph theory, and mathematical physics, yet numerous open questions remain. One central problem is the characterization of spectral invariants that uniquely determine a graph. Although isospectral but non-isomorphic graphs exist[28]. Extending this result to infinite or random graphs, as well as understanding the robustness of spectral invariants under perturbations, remains an important challenge. Similarly, stability and perturbation analysis of quantum graphs is an area of active research. Although local stability results exist for eigenvalues under small changes in edge lengths or vertex couplings[10, 51, 23, 42], sharp quantitative bounds and non-linear stability phenomena, particularly in random or leaky graphs, are still largely unexplored.

Another major direction is the study of randomness and universality. Quantum graphs provide a tractable model for testing conjectures from quantum chaos and Random Matrix Theory (RMT), yet a complete mathematical theory for universality in eigenvalue statistics remains elusive[26]. In particular, understanding how graph topology, such as bipartite versus non-bipartite structure, influences universality classes, and rigorously analysing resonance distributions and localization in disordered graphs, are open problems that combine combinatorial, probabilistic, and spectral analysis.

Quantum graphs also function as low-dimensional approximations of higher-dimensional systems, including thin manifolds and waveguides. Convergence theorems linking Laplacians on thin domains to quantum graph Hamiltonians exist[49], but several questions remain open. Extending these results to irregular or random geometries, developing precise error estimates for spectral quantities, and coupling quantum graphs with higher-dimensional PDE models are important challenges for both theory and applications. In parallel, the study of non-Hermitian and open quantum graphs has recently emerged as a frontier. Leaky graphs and transparent boundary conditions allow waves to escape the network, giving rise to complex resonances and exceptional points. Systematic theories for these phenomena and their applications to transport, photonics, and quantum information are still under development[17, 41].

Finally, quantum graphs offer significant potential in quantum technologies. Designing graph geometries that optimize spectral gaps for robust transport, developing graph-based models for quantum error correction, and extending quantum walk models into analytic frameworks for algorithmic applications are active areas of research[33]. Overall, these open problems illustrate that quantum graphs continue to occupy a unique position bridging deterministic spectral geometry, probabilistic models, and real-world applications. Progress on these challenges promises not only advances in pure mathematics but also practical impact on quantum networks, photonic devices, and nanoscale transport systems.

9. Conclusion

Quantum graphs stand at the intersection of analysis, geometry, and mathematical physics, offering a flexible structure that bridges discrete graph theory and continuous differential operators. They are essential for researching spectral theory and quantum chaos because of their precise solution capability in a variety of situations, most notably through secular equations and trace formulae. They offer rigorous analogues of phenomena that are otherwise only accessible through semi-classical approximations. Quantum graphs have provided significant insights into universal characteristics of quantum systems, ranging from eigenvalue statistics that align with random matrix theory to the intricate structure of nodal domains and spectral gaps.

Beyond their mathematical richness, quantum graphs play an increasingly important role in applications ranging from wave propagation in photonic networks to the design of nanoscale quantum devices and algorithms in quantum computation. At the same time, several open challengessuch as inverse spectral problems, non-linear extensions, and the modelling of open and leaky systemspoint to fertile ground for future research. Addressing these problems will not only advance spectral graph theory but also strengthen the connections between abstract mathematics and physical applications.

In conclusion, quantum graphs have matured into a central tool of modern mathematical physics. They provide both a rigorous theoretical laboratory for exploring quantum chaos and a practical framework for modelling real-world quantum systems. Continued interdisciplinary efforts promise to deepen our understanding of spectral phenomena and open new pathways in quantum technologies, ensuring that quantum graphs remain a vibrant area of mathematical and physical research for years to come.

References

[1] Alon, L., Band, R., & Berkolaiko, G. (2018). Nodal statistics on quantum graphs. Communications in Mathematical Physics, 362(3), 909-948. 5.2

[2] Alon, L., Band, R., & Berkolaiko, G. (2024). Universality of nodal count distribution in large metric graphs. Experimental Mathematics, 33(2), 301-335. 3.1

[3] Anantharaman, N., & Sabri, M. (2019). Quantum ergodicity on graphs: from spectral to spatial delocalization. Annals of Mathematics, 189(3), 753-835. 5.4

[4] Anderson, P. W. (1958). Absence of diffusion in certain random lattices. Physical review, 109(5):1492. 5.4387. 5.4

[5] Annoni, E., Frigerio, M., & Paris, M. G. (2024). Enhanced quantum transport in chiral quantum walks: E. Annoni et al. Quantum Information Processing, 23(4), 117. 6.3

[6] Avdonin, S. and Kurasov, P. (2008). Inverse problems for quantum trees. Inverse Probl. Imaging, 2(1):121. 5.2390. 5.2

[7] Band, R., & Charron, P. (2023). Sturm-Hurwitz Theorem for quantum graphs. arXiv preprint arXiv:2310.03877. 3.1

[8] Baptista, L., & Hofmann, M. (2025). On Courant-type bounds and spectral partitioning via Neumann domains on quantum graphs. arXiv preprint arXiv:2509.13228. 3.1

[9] Berkolaiko, G. (2013). Nodal count of graph eigenfunctions via magnetic perturbation. Analysis & PDE, 6(5), 1213-1233. 3.1

[10] Berkolaiko, G., & Kuchment, P. (2013). Introduction to quantum graphs (No. 186). American Mathematical Soc. 1, 3, 5.1, 8

[11] Berkolaiko, G., & Kuchment, P. (2022). Spectral shift via lateral perturbation. Journal of Spectral Theory, 12(1), 83-104. 5.4

[12] Berkolaiko, G., Schanz, H., & Whitney, R. S. (2003). Form factor for a family of quantum graphs: an expansion to third order. Journal of Physics A: Mathematical and General, 36(31), 8373-8392. 1

[13] Campbell, J., & Dooley, J. (2025). Optimization of Bottlenecks in Quantum Graphs Guided by Fiedler Vector-Based Spectral Derivatives. arXiv preprint arXiv:2506.07875. 3.2, 4.4

[14] Chung, F. R. (1997). Spectral graph theory (Vol. 92). American Mathematical Soc. 6.1

[15] Datta, S. (1997). Electronic transport in mesoscopic systems. Cambridge university press. 6.3

[16] Davies, E. B., Exner, P., & Lipovský, J. (2010). Non-Weyl asymptotics for quantum graphs with general coupling conditions. Journal of Physics A: Mathematical and Theoretical, 43(47), 474013. 5.1

[17] Exner, P. (2007). Leaky quantum graphs: a review. arXiv preprint arXiv:0710.5903. 1, 5.3, 8

[18] Exner, P. (Ed.). (2008). Analysis on Graphs and Its Applications: Isaac Newton Institute for Mathematical Sciences, Cambridge, UK, January 8-June 29, 2007 (Vol. 77). American Mathematical Soc. 4, 4.3

[19] Exner, P. (2011). Vertex couplings in quantum graphs: approximations by scaled Schrödinger operators. In Mathematics In Science And Technology: Mathematical Methods, Models and Algorithms in Science and Technology (pp. 71-92). 3.2

[20] Exner, P., & Post, O. (2005). Convergence of spectra of graph-like thin manifolds. Journal of Geometry and Physics, 54(1), 77-115. 6.2

[21] Exner, P., & Rohleder, J. (2025, April). Optimization of quantum graph eigenvalues with preferred orientation vertex conditions. In Annales Henri Poincaré (pp. 1-31). Cham: Springer International Publishing. 3.2, 4

[22] Exner, P., & Turek, O. (2007). Approximations of singular vertex couplings in quantum graphs. Reviews in Mathematical Physics, 19(06), 571-606. 1, 4.1, 4.2

[23] Fulling, S. A. (2005). Local spectral density and vacuum energy near a quantum graph vertex. arXiv preprint math/0508335. 8

[24] Georgescu, C. A., Schalkers, M. A., & Möller, M. (2025). qlbmA quantum lattice Boltzmann software framework. Computer Physics Communications, 315, 109699. 7

[25] Ghutishvili, T., Chen, L., Anlage, S. M., & Antonsen, T. M. (2023). Impedance statistics of cable networks that model quantum graphs. Physical Review Research, 5(3), 033195. 4, 4.1, 4.3, 4.4

[26] Gnutzmann II, S., & Smilansky, U. (2006). Quantum graphs: Applications to quantum chaos and universal spectral statistics. Advances in Physics, 55(5-6), 527-625. 1, 3, 8

[27] Goodman, R. H., Conte, G., & Marzuola, J. L. (2025). QGLAB: A MATLAB package for computations on quantum graphs. SIAM Journal on Scientific Computing, 47(2), B428-B453. 7

[28] Gutkin, B., & Smilansky, U. (2001). Can one hear the shape of a graph?. Journal of Physics A: Mathematical and General, 34(31), 6061-6068. 5.2, 8

[29] Harrell II, E. M., & Maltsev, A. V. (2024). On topological bound states and secular equations for quantum-graph eigenvalues. Journal of Spectral Theory, 14(2), 619-639. 4, 4.2

[30] Hofmann, M., Kennedy, J. B., Mugnolo, D., & Plümer, M. (2021, November). On Pleijels nodal domain theorem for quantum graphs. In Annales Henri Poincaré (Vol. 22, No. 11, pp. 3841-3870). Cham: Springer International Publishing. 3.1

[31] Ingremeau, M. (2022). Scattering resonances of large weakly open quantum graphs. Pure and Applied Analysis, 4(1), 49-83. 4, 4.2

[32] Ingremeau, M. (2022). A trace formula for scattering resonances of unbalanced quantum graphs. arXiv preprint arXiv:2206.12460. 4, 4.2

[33] Kempe, J. (2003). Quantum random walks: an introductory overview. Contemporary Physics, 44(4), 307-327. 8

[34] Kennedy, J. (2024). Geometric spectral theory of quantum graphs. Communications in Mathematics, 32. 3

[35] Kostrykin, V., & Schrader, R. (1999). Kirchhoff's rule for quantum wires. Journal of Physics A: Mathematical and General, 32(4), 595-630. 2.2, 4.1

[36] Kottos, T., & Smilansky, U. (1997). Quantum chaos on graphs. Physical review letters, 79(24), 4794. 3

[37] Kottos, T., & Smilansky, U. (1999). Periodic orbit theory and spectral statistics for quantum graphs. Annals of Physics, 274(1), 76-124. 1, 3.3, 4.4

[38] Kuchment, P. (2003). Quantum graphs: I. Some basic structures. Waves in Random media, 14(1), S107. 1, 4, 4.3

[39] Kuchment, P. (2005). Quantum graphs: II. Some spectral properties of quantum and combinatorial graphs. Journal of Physics A: Mathematical and General, 38(22), 4887-4900. 3.2, 5.3, 6.1

[40] Kurasov, P. (2024). Spectral geometry of graphs (p. 639). Springer Nature. 5.1

[41] Lavrukhine, A. A., Popov, A. I., & Popov, I. Y. (2023). On transparent vertex boundary conditions for quantum graphs: AA Lavrukhine et al. Indian Journal of Physics, 97(7), 2095-2102. 8

[42] awniczak, M., Kurasov, P., Bauch, S., Biaous, M., Akhshani, A., & Sirko, L. (2021). A new spectral invariant for quantum graphs. Scientific Reports, 11(1), 15342. 8

[43] Matsuda, J. (2024). Algebraic connectedness and bipartiteness of quantum graphs. Communications in Mathematical Physics, 405(8), 185. 3

[44] Miroshnichenko, A. E., Flach, S., & Kivshar, Y. S. (2010). Fano resonances in nanoscale structures. Reviews of Modern Physics, 82(3), 2257-2298. 6.4

[45] Mohseni, M., Rebentrost, P., Lloyd, S., & Aspuru-Guzik, A. (2008). Environment-assisted quantum walks in photosynthetic energy transfer. The Journal of chemical physics, 129(17). 6.4

[46] Pauling, L. (1936). The diamagnetic anisotropy of aromatic molecules. The Journal of chemical physics, 4(10), 673-677. 1

[47] Pauling, L. (1992). The nature of the chemical bond1992. Journal of Chemical Education, 69(7), 519. 6.4

[48] Plümer, M., & Täufer, M. (2021). On fully supported eigenfunctions of quantum graphs. Letters in Mathematical Physics, 111(6), 153. 3.1

[49] Post, O. (2012). Spectral analysis on graph-like spaces (Vol. 2039). Springer. 6.2, 8

[50] Silva, A. A., Bazeia, D., & Andrade, F. M. (2025). Entangled states from simple quantum graphs. Journal of Physics A: Mathematical and Theoretical, 58(43), 43LT01. 6.3

[51] Sofer, G. (2022). Spectral curves of quantum graphs with δ_s type vertex conditions. arXiv preprint arXiv:2212.09143. 8

[52] Yu, Y. C., & Cai, X. (2023). Controlled transport in chiral quantum walks on graphs. New Journal of Physics, 25(8), 083034. 6.3