1

Introduction

This chapter provides a historical introduction. Spectra first appeared in the study of linear differential operators, such as the Laplace, the heat, and the wave operator, which originated in the eighteenth century. A Laplace operator on networks was first introduced by Kirchhoff in the nineteenth century.

1.1 Linear Partial Differential Equations, the Classical Laplace Operator, and Eigenvalue Problems

In recent decades, many empirical structures have been described as networks that is, constituted by (possibly weighted and/or directed) relations between basic constituents or elements. In fact, network analysis is a well-established subject within the general theory of complex systems, and quite a number of monographs have been devoted to it, besides an enormous number of research papers in several different disciplines. Mathematically, such a network is described as a (possibly weighted and/or directed) graph, or perhaps as a more general structure such as a simplicial complex or a hypergraph. The resulting graphs, however, typically are less regular or possess less structure than those traditionally studied in graph theory. Also, they can be quite large, if not sometimes gigantic. Since computational approaches to problems such as subgraph isomorphism tend to be difficult and often NP hard or even complete [65, 235, 242], efficient techniques are needed to study these empirical structures. One such approach includes the introduction of a some linear operator defined in terms of the network structure that operates on functions defined on the vertices. As a linear operator, it possesses a spectrum consisting of finitely many eigenvalues, as the structure, while possibly large, is finite. And when the operator is symmetric, these eigenvalues are real. The computation of the eigenvalues of symmetric linear operators is computationally relatively easy,

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and there exist fast algorithms that can produce the spectrum, or some relevant parts of it, for quite large networks. The question is what this spectrum can tell us about the underlying network. One quickly realizes that there are so-called graphs, that is, non-isomorphic graphs that nevertheless have the same spectrum, and therefore the spectrum cannot recover the graph completely. Nevertheless, as we shall explore in this monograph, many important qualitative properties of the underlying graph can be inferred from its spectrum. And perhaps we may not even be interested in all details, as empirical networks usually possess a certain amount of randomness, resulting from the stochastic process that brought them into being, such as biological evolution. While, as mentioned, such empirical networks tend to be less regular, more diffuse, partly random, and in any case qualitatively different from those preferred by many graph theorists, there exists an important mathematical paradigm that has become fundamental for mathematical approaches to network analysis. This refers to the 1959 paper [91] by Paul Erdős and Alfréd Rényi that introduced the concept of a random graph [91] and derived and explained several of its characteristic properties. The Book [32] is a systematic presentation of the theory of random graphs. More recently, other types of random networks were introduced that seem to match some of the features better than that are typically found in empirical networks. Since here we present a general approach to the spectral analysis of such structures, these details are not so important for our purposes.

The spectral theory of linear operators is a wide subject, with diverse sources from mathematics and physics and with ramifications into many different, perhaps almost all, mathematical fields. Even though the setting that we adopt in this book is more confined and the basic story has nothing to do with network analysis, it might be useful to provide a wider historical perspective.

The story might start with the introduction of the wave operator, also called the d'Alembertian, by Jean-Baptiste Le Rond d'Alembert (1717–83) in 1747. We can follow the account of the story given by Bernhard Riemann (1826–66) in his habilitation thesis (see pp. 227–271 in [236]) (profound historical information can also be found in [80]). D'Alembert was the first mathematician to formulate a partial differential equation. He postulated that for a vibrating string, modeled as a one-dimensional line of length ℓ, its extension $y(x,t)$ at time t, that is, its deviation from rest, on the interval $x \in [0,\ell]$ satisfies the following differential equation:

$$\frac{\partial^2 y}{\partial t^2} = \alpha^2 \frac{\partial^2 y}{\partial x^2}, \tag{1.1.1}$$

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where α is independent of t, and also of x, if the string is uniformly thick. D'Alembert found that the general solution is given by

$$f(x+\alpha t)+g(x-\alpha t) \tag{1.1.2}$$

by introducing the variables $\xi = x+\alpha t$ and $\eta = x-\alpha t$ and rewriting (1.1.1) as

$$4\frac{\partial^2 y}{\partial \xi \partial \eta} = 0. \tag{1.1.3}$$

This led to a dispute with Leonhard Euler (1707–83) about which types of functions f and g should be admitted in (1.1.2), with d'Alembert insisting that the functions should be analytic. Later, Daniel Bernoulli (1700–82) entered the debate and proposed to consider solutions of the form

$$y = \sum a_k \sin\frac{k\pi x}{\ell}\cos\frac{k\pi\alpha(t-\beta_k)}{\ell}. \tag{1.1.4}$$

(It is assumed that the string is fixed at its endpoints, that is, $y(0,t) = y(\ell,t) = 0$.)

But Euler argued at the time that a sum of analytic functions could not represent general functions of the form (1.1.2), and therefore Bernoulli's approach was more restricted than his own. Then, also the young Joseph-Louis Lagrange (1736–1813) entered the debate, but a solution had to wait for almost 50 years until Jean-Baptiste Joseph Fourier (1768–1830) proposed his general theory of series expansions in terms of trigonometric functions. A mathematically rigorous proof of such an expansion for a general class of functions was subsequently provided by Peter Gustav Lejeune Dirichlet (1805–59). For the general solution, Riemann developed the modern theory of integration, which was continued by Henri Lebesgue (1875–1941). The Lebesgue integral enabled mathematicians to define the spaces $L^p(\Omega)$ of functions whose p-th power is integrable on some domain Ω. Importantly, these spaces are complete with respect to the corresponding norm. This made the development of modern functional analysis possible, with the fundamental concept of a Banach space. In particular, we have the Hilbert space $L^2(\Omega)$, which is indispensable for the mathematical formulation of quantum mechanics.

In a somewhat different direction, the analysis of the set of points where a Fourier series might not converge ultimately led Georg Cantor (1845–1918) to the creation of modern set theory.

But what does all that have to do with spectra? The answer is easy. When we try to compute a solution of (1.1.1) by separation of variables, that is, make the ansatz

$$y(x,t) = h(x)\phi(t), \tag{1.1.5}$$

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the equation becomes, using now subscripts for partial derivatives,

$$h(x)\phi_{tt}(t) = \alpha^2\phi(t)h_{xx}(x). \tag{1.1.6}$$

Therefore,

$$\frac{h_{xx}(x)}{h(x)} = \frac{1}{\alpha^2}\frac{\phi_{tt}(t)}{\phi(t)} \tag{1.1.7}$$

both have to be constant. When we substitute the value of this constant as $-\lambda$, we obtain the following eigenvalue equation:

$$-h_{xx}(x) = \lambda h(x). \tag{1.1.8}$$

On the interval $[0,\ell]$ with the boundary conditions $h(0) = 0 = h(\ell)$, (1.1.8) is satisfied by the following trigonometric functions:

$$h(x) = \sin\frac{n\pi x}{\ell}, \tag{1.1.9}$$

for the values

$$\lambda = \left(\frac{n\pi}{\ell}\right)^2. \tag{1.1.10}$$

Thus, in modern terminology, the functions (1.1.9) are the eigenfunctions of the operator $-h_{xx}$, the values (1.1.10) are the eigenvalues, and the Fourier expansion justifying Bernoulli's solution (1.1.4) is simply an expansion in terms of the eigenfunctions of the operator $-h_{xx}$. The eigenvalues (1.1.10) then represent the possible vibration modes of the string.

When we have vibrations of objects described by more than one spatial dimension, we obtain the wave equation as follows:

$$\frac{\partial^2 y}{\partial t^2} = -\alpha^2\Delta y(x,t), \tag{1.1.11}$$

with the operator

$$-\Delta h(x) = \sum_{i=1}^{n}\frac{\partial^2 h}{\partial(x^i)^2}(x), \tag{1.1.12}$$

for $x = (x^1,\ldots,x^n)$. The minus sign in (1.1.12) is historically incorrect, but in line with the conventions adopted in this book. The operator $(-)\Delta$ is called the *Laplace operator*, or more shortly, the *Laplacian*, although it was first introduced and studied by Lagrange [129]. It played a fundamental role in Laplace's *Celestial Mechanics*.

For a solution of (1.1.11), we may again propose a separation of variables, as follows:

$$y(x,t) = h(x)\phi(t), \tag{1.1.13}$$

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and the equation becomes

$$h(x)\phi_{tt}(t) = -\alpha^2\phi(t)\Delta h(x). \tag{1.1.14}$$

Therefore,

$$\frac{-\Delta h(x)}{h(x)} = \frac{1}{\alpha^2}\frac{\phi_{tt}(t)}{\phi(t)} = -\lambda \tag{1.1.15}$$

for a constant λ. We obtain the following eigenvalue equation:

$$\Delta_{xx}(x) = \lambda h(x), \tag{1.1.16}$$

for the Laplace operator, which, for given boundary conditions on a bounded domain, again has nontrivial solutions only for a discrete set of eigenvalues $\lambda \geq 0$. As before, a general solution of (1.1.11) can be expanded in terms of the eigenfunctions of Δ. The eigenvalues and eigenfunctions depend on the geometry of the domain Ω, and therefore in general can no longer be written in terms of trigonometric functions (unless Ω is of a rectangular form $[0,\ell_1]\times\ldots\times[0,\ell_n]$), but the principle of an expansion of a solution of a linear differential equation in terms of eigenfunctions remains the same.

Fourier had considered the heat equation:

$$\frac{\partial y}{\partial t} = -\Delta y(x,t), \tag{1.1.17}$$

but the principle of an expansion in terms of eigenfunctions of $-\Delta$ applies here as well.

In this book, we shall investigate this principle not for differential operators on Euclidean (or more general) domains, but rather for difference operators on discrete structures. But before we get into that, we should discuss some other historical strands.

When Bernhard Riemann had introduced the concepts of Riemannian geometry in his habilitation address [237, 238], Eugenio Beltrami (1835–1900) realized that in Riemannian geometry, there is a natural analog of the Laplace operator. This operator is now called the Laplace–Beltrami operator. Like the Laplace operator, it operates on functions, now defined on Riemannian manifolds. A further important generalization emerged when operating with differential forms. Élie Cartan (1869–1951) had used the exterior algebra created by Hermann Graßmann (1809–77) to develop a calculus of differential forms. When ω is a p-form, that is, in local coordinates, a linear combination of expressions of the type $\eta(x)dx^{i_1}\wedge\ldots\wedge dx^{i_p}$, one can define its differential $d_p\omega$, which for this expression is the $(p+1)$-form,

$$d_p\eta(x)dx^{i_1}\wedge\ldots\wedge dx^{i_p} = \sum_j \frac{\partial\eta(x)}{\partial x^j}dx^j\wedge dx^{i_1}\wedge\ldots\wedge dx^{i_p}. \tag{1.1.18}$$

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Since the Riemannian metric induces a natural scalar product on q-forms, one has an adjoint operator $d_p^\star$ mapping a $(p+1)$-form to a p-form, and one considers the operator,

$$\Delta_p = d_{p-1}d_{p-1}^\star + d_p d_p^\star. \tag{1.1.19}$$

This operator is called the *Hodge Laplacian*, but the theory was developed more or less simultaneously and independently by Hermann Weyl (1885–1955), Georges de Rham (1903–90), William Hodge (1903–75), and Kunihiko Kodaira (1915–97). For $p = 0$ (where $d_{-1} = 0$), it becomes the Laplace–Beltrami operator, which, when the metric is Euclidean, is the Laplace operator. Beno Eckmann (1917–2008) then introduced a combinatorial operator that is analogous to Δ_p for simplicial complexes. The eigenvalues of all these operators, the Laplace operator on a domain in Euclidean space, the Laplace–Beltrami operator on a Riemannian manifold, the Hodge Laplacian on differential forms, or the Eckmann Laplacian on simplicial complexes, all encode important geometric information about the underlying spaces.

But before we come to that, the reader may have wondered about the origin of the terms *eigenvalue* and *eigenfunction*.

While Gottfried Wilhelm Leibniz (1646–1716) had already introduced the determinant of a matrix, and linear algebra in Cartesian spaces had been developed by Arthur Cayley (1825–91) and Graßmann, but was generally accepted only much later, it was the theory of integral equations that ultimately led to general spectral theory. When David Hilbert (1862–1943) learned about the work of Erik Ivar Fredholm (1866–1927) on general integral equations, he realized that for symmetric equations, a much richer theory could be developed. This led to the analysis of compact linear operators in Hilbert spaces in terms of their spectra, that is, the collection of their eigenvalues, and more generally, to bounded or even unbounded such operators. It turned out that this provided the appropriate mathematical framework for developing the quantum mechanics discovered by Werner Heisenberg (1901–76) and Erwin Schrödinger (1887–1961), at the hands of John von Neumann (1903–57). There, operators represent quantum mechanical observables, and their eigenvalues are the possible outcomes of observations. Also, the Schrödinger equation is naturally studied on spaces of complex-valued functions in the Hilbert space L^2. And this is true more generally for linear partial differential equations, such as the Laplace equation $\Delta y = 0$, the heat equation (1.1.17), and the wave equation (1.1.11), where Fourier expansions converge in Hilbert spaces. And the terms *eigenvalue* and *eigenfunction*, to finally come to that, are derived from Hilbert's German expressions *Eigenwert* and *Eigenfunktion* in

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[134]. (The German *eigen* means *proper, particular, characteristic, and inherent*.) A curious anecdote highlights the humorous misunderstanding that they were named after the biophysical chemist and Nobel laureate Manfred Eigen (1927–2019).

1.2 Laplace-Type Operators on Graphs

The theory of linear partial differential equations, Fourier expansions, or linear operators in Hilbert spaces had to overcome many analytical obstacles for their successful development and applications. In particular, it took a long time before mathematicians had developed the appropriate versions of convergence and could successfully apply them in those theories. In this book, however, we treat a situation that faces none of these analytical difficulties. We consider Laplace-type operators on finite discrete structures, such as graphs, simplicial complexes, or hypergraphs. Strangely, the corresponding theory was developed much later than its analytical analog just described, and it really got off the ground only when it became inspired by the latter.

Nevertheless, there does exist an origin from the nineteenth century. In 1847, Gustav Kirchhoff (1824–87) introduced a discrete version of the Laplace operator, for the study of electrical networks [140, 173]. He defined the operator of a graph with adjacency matrix A and diagonal degree matrix D as

$$K := D - A. \tag{1.2.1}$$

Here, for a graph with N vertices, the adjacency matrix has entry $a_{vv'} = 1$ when the vertices $v \neq v'$ are connected by an edge, and $a_{vv'} = 0$ else, and the degree of vertex v is $\deg_v = \sum'_v a_{vv'}$. (This is for an unweighted graph; in a weighted graph, we can consider $a_{vv'}$ as the weight of the edge from v to v'.) The spectrum of this operator has been widely studied in algebraic graph theory (see, for instance, [29, 38, 72]).

While this operator can be seen as a discrete version of the Laplace operator, a version that is a better analog in many respects is the Chung Laplacian, as follows:

$$\mathcal{L} := \mathrm{Id} - D^{-1/2} A D^{-1/2}, \tag{1.2.2}$$

where Id is the $N \times N$ identity matrix. This operator was first systematically studied by Fan Chung [61]. For instance, $\mathcal{L}$ is the operator that generates random walks on the graph, in the sense of [68] (see [146]). Putting

$$\Delta := D^{-1/2} \mathcal{L} D^{1/2}, \tag{1.2.3}$$

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the matrices Δ and $\mathcal{L}$ become similar, which implies that they have the same spectrum, that is, the same eigenvalues counted with multiplicity. While K in (1.2.1) and the operator (1.2.2) are obviously symmetric operators, the operator (1.2.3) is also symmetric with respect to some scalar product (see [145]), as will become clear below, see (4.1.32).

As already indicated several times, the general question is what the spectrum of some Laplace operator, be it a continuous or a discrete one, can tell us about the underlying structure. For example, what can we learn from the spectrum of the Laplace operator operating on functions that vanish on the boundary of some bounded domain in $\mathbb{R}^n$ about the geometry of that domain? Or what can we learn from the spectrum of the Laplace–Beltrami operator on a compact Riemannian manifold about the geometry of that manifold? Or what can the spectrum of (1.2.1) or (1.2.2) tell us about the structure of the underlying finite graph?

In fact, in 1882, the physicist Arthur Schuster (1851–1934)[47] put forth a question: *Can one determine the shape of an object by listening to its vibrations?* Mark Kac [164] famously reformulated it as: *Can one hear the shape of a drum?* But recalling the previous discussion of the wave operator and the expansion of its solutions by Bernoulli and Fourier, the question was modified as: *Can one reconstruct the shape of a mathematical drum from the eigenvalues of its Laplace operator?*, where *mathematical drum* stands for a Euclidean domain. A negative answer was given in 1992 by Carolyn Gordon, David L. Webb, and Scott Wolpert in a paper titled "One cannot hear the shape of a drum" [114]. In other words, one cannot reconstruct the exact shape of an object from the eigenvalues of the Laplacian. Nevertheless, one can infer important information. In 1911, Weyl [272] proved an asymptotic formula for the eigenvalues of a bounded domain in terms of its dimension and volume, and Weyl's reasoning directly extends to Riemannian manifolds. In fact, in 1953, Minakshisundaram [209] showed that for a compact Riemannian manifold without boundary, one can hear the dimension, the volume, and the total scalar curvature (see, for instance, [47]). The situation for the discrete Laplacians on graphs is analogous.

The results of Weyl use the asymptotics of the spectrum, that is, the large eigenvalues. But even a single small eigenvalue, in fact the first positive eigenvalue, can reveal important geometric features. Again, this started in the context of continuous problems. While the general idea of relating isoperimetric and Sobolev inequalities emerged already in [94, 204], the decisive step was taken by Cheeger [56] in Riemannian geometry. For a compact, connected n-dimensional manifold M, he defined

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$$h(M) \coloneqq \inf_{D} \frac{\mathrm{vol}_{n-1}(\delta D)}{\mathrm{vol}_n(D)},$$

where $D \subset M$ is a smooth n-submanifold with boundary δD and $0 < \mathrm{vol}_n(D) \leq \mathrm{vol}(M)/2$. Cheeger proved that the first nonvanishing eigenvalue $\lambda_{\min}(M)$ of the Laplace–Beltrami operator satisfies

$$\lambda_{\min}(M) \geq \frac{1}{4} h^2(M).$$

Peter Buser [41] later showed that for each compact manifold, there exists Riemannian metrics for which the inequality becomes sharp. In [42], he also proved that if the Ricci curvature of a compact unbordered Riemannian n-manifold M is bounded below by $-(n-1)a^2$, for some $a \geq 0$, then

$$\lambda_{\min}(M) \leq 2a(n-1)h + 10h^2.$$

Therefore, $h(M)$ can be used to estimate $\lambda_{\min}(M)$ and vice versa.

It was then discovered that an analogous relation holds for the Laplacian of a graph. In fact, what is now called the *Cheeger constant* of a simple graph $G = (V, E)$ with vertex set V and edge set E had already been introduced in 1951 by George Pólya and Gábor Szegö [230], who called it the *isoperimetric constant* and defined it as

$$h(G) \coloneqq \min_{\emptyset \neq S \subseteq V} \frac{|E(S, \bar{S})|}{\min\{\mathrm{vol}(S), \mathrm{vol}(\bar{S})\}},$$

where $E(S, \bar{S})$ denotes the set of edges between S and its complement $\bar{S} \coloneqq V \setminus S$, while the *volume* of S, denoted $\mathrm{vol}(S)$, is the sum of the vertex degrees in S. Finding a set S realizing the Cheeger constant, also called a Cheeger cut, means finding a small *edge cut* $E(S, \bar{S})$ such that, if removed from G, it divides the graph into two disconnected components that have roughly equal volume. Therefore, h measures how different G is from a disconnected graph, and it is largest for the complete graph.

Jozef Dodziuk [82] and Noga Alon with Vitali Milman [4] derived analogous estimates for the graph Cheeger constant and for the first nonvanishing eigenvalue of the Kirchhoff Laplacian (1.2.1) associated to a connected graph. Also, Fan Chung [61] proved the Cheeger inequalities for the *symmetric Chung Laplacian* (1.2.2) of a graph. Chung's estimate reads as

$$\frac{1}{2} h(G)^2 \leq \lambda_2(G) \leq 2h(G), \tag{1.2.4}$$

where $\lambda_2(G)$ is the first nonzero eigenvalue of the connected graph G (the first eigenvalue is always $\lambda_1(G) = 0$, for a constant eigenfunction). Thus, as in the Riemannian case, $h(G)$ can be used to estimate $\lambda_2(G)$ and vice versa.

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Moreover, the eigenvectors corresponding to $\lambda_2(G)$ can be used in order to approximate the Cheeger cut, as follows. An eigenvector for $\mathcal{L}(G)$ can be seen as a function $f\colon V \to \mathbb{R}$ and, if f is an eigenfunction with eigenvalue $\lambda_2(G)$, then f must achieve both positive and negative values, and the edges between the sets

$$\{v \in V\colon f(v) \geq 0\} \quad \text{and} \quad \{v \in V\colon f(v) < 0\}$$

approximate the Cheeger cut. Since solving the Cheeger cut problem is NP-hard [256], while the eigenvalues and the eigenvectors of $\mathcal{L}(G)$ can be found quickly, spectral clustering based on these results is a very common tool and has many applications (see, for instance, [49, 53, 253, 270, 271]).

1.3 Other Sources and Directions of the Theory

Like most other mathematical subjects, the spectral theory of discrete structures has multiple origins and expands into different research directions, besides those that we have cited for the history and that we develop in this book. Thus, it seems appropriate to sketch those that are perhaps the most important ones.

An important source was the paper [199] by Grigorii Aleksandrovich Margulis where he found an explicit construction of an infinite family of graphs, which are what he called *concentrators* and which are, with a shift of emphasis, now called *expanders*. Mark Pinsker [229] had already shown the existence of such graphs by a probabilistic argument. Concentrators are graphs where there exist many disjoint paths from any set of k inputs to k outputs. Expanders are graphs for which every subset of a vertex set has a large neighborhood. This means that many edges have to lead from that subset to its complement. Expanders can be used to construct superconcentrators [102]. See also the discussion in [61]. In either case, the graph should be sparse, that is, not have many edges. Such families of graphs are important in computer science, for instance, for efficient network communication. Other applications include error-correcting codes, cryptography, or complexity theory. We shall discuss this in Section 13.3. In that theory, one is mainly interested in d-regular graphs, that is, in graphs where all vertices have the same number d of neighbors. It turns out that if one wishes to make the expansion property quantitative, a good measure is a lower bound for the smallest nonvanishing eigenvalue λ_2 of the Laplace operator. The lower bound in (1.2.4) here explains why this is so. As mentioned earlier, the subject will be taken up in Section 13.3, but here we

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refer to [136, 176, 192]. In fact, this is a well-researched field with a rather extensive literature.

Since the d-regularity of the graphs makes the graphs more regular and uniform, one can also profitably invoke many other mathematical areas and apply their tools. In fact, Margulis' original construction was of a number theoretic nature, and subsequently, again by number theoretical ideas, other classes of expander graphs have been found, such as the Ramanujan graphs. For a number and group theoretical survey, see [193].

An important topic is that of *random graphs*. The basic construction was introduced by Paul Erdös (1913–96) and Alfred Rényi (1921–70) [91]. Given a set of N vertices, and some $p \in (0,1)$, every pair of vertices is connected by an edge with probability p, independently of other pairs. The typical properties of such random graphs scale like $\frac{p}{N}$. They have been intensively studied (see, for instance, [32]). Also, their spectra have many interesting features (see, for instance, [136]). Random constructions can also be used for proving the existence of graphs with certain specified properties, but such constructions do not provide explicit examples.

Another direction that is complementary to what we cover in this book is the spectral geometry of infinite graphs. This topic also involves important analytical aspects, such as the heat flow on the underlying graph, and it is advantageously treated from the general perspective of Dirichlet forms. Here, we refer to the recent comprehensive monograph [171].

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