A SURVEY ON SPECTRA OF INFINITE GRAPHS

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Contents

1. *Introduction*

In the last decade, considerable attention has been paid by graph theorists to the study of spectra of graphs and their interaction with structure and characteristic properties of graphs. After the 'classical' book by N. L. Biggs [12] on algebraic graph theory in general, the first comprehensive monograph on this particular topic, by D. M. Cvetković, M. Doob and H. Sachs [34], appeared in 1979. It dealt exclusively with finite graphs. In a recent article by the first two authors [32], a survey of new developments is given, including a short section on infinite graphs. On the other hand, spectral theory of graphs, in particular infinite graphs, and related topics have been dealt with to a considerable extent 'disguised' in the framework of the theory of non-negative matrices, harmonic analysis on graphs and discrete groups (Cayley graphs), analytic probability theory, Markov chains and other mathematical branches. In fact, some results have been rediscovered several times under different viewpoints.

The purpose of this survey is to give an overview of results on spectra of infinite graphs, emphasizing how contributions from different areas fit into this graph-theoretical setting. For the moment, we point out the books by E. Seneta [113] and by A. Figà-Talamanca and M. A. Picardello [45] as two examples. Among the variety of books on the background in functional analysis and matrix theory, we emphasize [1, 30, 41, 118, 129]. Our approach follows that of B. Mohar [89] and related definitions of spectra, as they have been used in the mathematical fields mentioned above. A different approach, due to A. Torgašev [119], will be only briefly discussed; the reader is referred to the recent book [33].

Primarily, this survey is addressed to graph theorists; there also is some emphasis on 'spectral' properties of random walks on graphs. The selection of those topics which can (or should) in some way be regarded in connection with spectral theory of graphs could most likely be extended towards infinity. Therefore, the present survey is biased by the viewpoint of the authors and cannot be complete. We apologize to all those who feel that their work is missing in the references or has not been emphasized sufficiently in the text.

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2. *Linear operators associated with a graph*

Let $G = (V, E)$ be an unoriented graph, finite or countably infinite, possibly having loops and multiple edges, and let $\mathbf{B}(G) = \mathbf{B} = (b_{u,v})_{u,v \in V}$ be a (real or complex) square matrix indexed by the vertices of G. If G is finite, the set of all eigenvalues of $\mathbf{B}$ is called the $\mathbf{B}$-*spectrum* of the graph. Various ways of associating matrices with finite graphs and the corresponding spectra are treated in [34]. If G is infinite, the spectrum of $\mathbf{B}(G)$, denoted by $\mathrm{spec}\,(\mathbf{B}(G))$, depends on the choice of a suitable space on which $\mathbf{B}$ acts as a linear operator. Usually, one considers the Hilbert space $l^2(V)$. It can also be replaced by any of the spaces $l^p(V)$, consisting of all complex column vectors

$$\mathbf{x} = (x_v)_{v \in V} \tag{2.1}$$

satisfying

$$\|\mathbf{x}\|_p = (\sum_{v \in V} |x_v|^p)^{1/p} < \infty, \tag{2.2}$$

where $1 \leqslant p < \infty$; for $p = \infty$, the norm reduces to $\|\mathbf{x}\|_\infty = \max \{|x_v| \,|\, v \in V\}$. The action of $\mathbf{B}$ is matrix multiplication: the coordinates of $\mathbf{y} = \mathbf{Bx}$ are

$$y_u = \sum_{v \in V} b_{u,v} x_v, \quad u \in V, \tag{2.3}$$

whenever these series converge. Linked with the problem of convergence is the choice of the appropriate definition range of $\mathbf{B}$; see §3. One may also consider the action of $\mathbf{B}$ on the space of *all* complex (in particular, positive; see §6) vectors over V; this is well defined in most cases. We now describe several ways to associate a matrix $\mathbf{B}(G)$ with a graph G, further details will be discussed in the following sections.

The most natural choice is the *adjacency matrix* $\mathbf{A} = \mathbf{A}(G)$; see [12, 34, 89]. For $u, v \in V$, its entry $a_{u,v}$ is the number of edges between u and v; in particular, $a_{u,u}$ is the number of loops at u. Here, one has to assume that G is *locally finite*: $\deg(u) < \infty$ for every vertex u, where $\deg(u)$ is the number of edges emanating from u. If $\deg(G) = \sup \{\deg(u) \,|\, u \in V\} < \infty$, then $\mathbf{A}$ acts on $l^2(V)$ as a self-adjoint operator with norm at most $\deg(G)$.

Another very common matrix associated with a *locally finite* graph G is the *transition matrix* $\mathbf{P} = \mathbf{P}(G) = (p_{u,v})_{u,v \in V}$, where

$$p_{u,v} = a_{u,v}/\deg(u). \tag{2.4}$$

This is a stochastic matrix (all row sums equal one), and as such it gives rise to a Markov chain with state space V, usually called *simple random walk* (*SRW*) on G [39, 55, 116]: the SRW is a sequence $X_n, n = 0, 1, 2, \ldots$, of V-valued random variables which have the Markov property

$$\mathrm{Pr}\,[X_n = v \,|\, X_k = u_k, k = 0, 1, \ldots, n-1] = \mathrm{Pr}\,[X_n = v \,|\, X_{n-1} = u]$$

$$= p_{u,v} \quad \text{for all } u_0, u_1, \ldots, u_{n-1} = u, v \in V. \tag{2.5}$$

Thus, X_n is the random position at time n, and we move along the edges according to probabilities $p_{u,v}, u, v \in V$. The transition matrix acts as a self-adjoint operator with norm bounded by one on the Hilbert space $l^2_\#(V)$ of all vectors $\mathbf{x}$ with

$$\|\mathbf{x}\|_{2,\#} = \langle \mathbf{x}, \mathbf{x} \rangle_\#^{\frac{1}{2}} < \infty, \tag{2.6}$$

where the inner product is given by

$$\langle \mathbf{x}, \mathbf{y} \rangle_{\#} = \sum_{v \in V} x_v \overline{y_v} \deg(v); \tag{2.7}$$

see, for example, [75, 102]. Note that G is assumed to be locally finite, but we do not demand here that $\deg(G) < \infty$.

Associated with each of the preceding two matrices are the *difference Laplacians*

$$\Delta_A(G) = \mathbf{D}(G) - \mathbf{A}(G) \tag{2.8}$$

and

$$\Delta_P(G) = \mathbf{I}(G) - \mathbf{P}(G), \tag{2.9}$$

where $\mathbf{D}(G)$ is the diagonal matrix $\mathrm{Diag}(\deg(v), v \in V)$ and $\mathbf{I}(G)$ is the identity matrix over V; compare, for example, with [35, 37].

If G is *regular* (*homogeneous*), that is, all vertices have the same degree, then results for $\mathbf{A}(G)$ carry over to $\Delta_A(G)$ and also to $\mathbf{P}(G)$ and $\Delta_P(G)$, dividing by $\deg(G)$ (and vice versa).

Finally, a completely different approach is due to A. Torgašev [119]. Consider a graph G without multiple edges. Choose a constant $\mathbf{a}, 0 < \mathbf{a} < 1$, and a labelling $V = \{v_1, v_2, v_3, \ldots\}$ of the vertex set, and define the matrix $\mathbf{C} = \mathbf{C_a} = (c_{i,j})_{i,j \in \mathbb{N}}$ by

$$c_{i,j} = a_{v_i, v_j} \cdot \mathbf{a}^{i+j-2}. \tag{2.10}$$

Then $\mathbf{C}$ gives rise to a self-adjoint compact operator on $l^2(V)$, which is Hilbert–Schmidt and hence allows the use of a well-developed spectral theory. In particular, there is no need to assume local finiteness of G. On the other hand, the spectrum depends both on labelling and parameter $\mathbf{a}$, and there seem to be no natural choices available.

Many details and references concerning Torgašev's method can be found in [32, 33], so that we shall not go into further details of this part of the theory.

For the rest of this paper, we shall always assume that G is an infinite, locally finite graph.

3. *Basic results*

The adjacency matrix $\mathbf{A} = \mathbf{A}(G)$ of G acts on vectors in $l^2(V)$ as described in (2.3). Its action is well-defined on all vectors which have only finitely many nonzero entries, and these form a dense subspace of $l^2(V)$. The operator with this definition range is symmetric and thus closeable. Its closure is called the *adjacency operator* of G, and will be denoted by the same symbol $\mathbf{A}$ as the adjacency matrix. This operator has self-adjoint extensions, but they are not unique in general. It is known [93] that there are infinite graphs with deficiency index n for any $n \geqslant 0$ (see [41] for the definition). An example of a graph with no unique self-adjoint extension was independently given in [100]. The self-adjoint extension is unique only if the deficiency index equals zero. This is the case when $\deg(G) < \infty$, as we have the following theorem (see [89]).

THEOREM 3.1.   *The adjacency operator is bounded (and thus everywhere defined and self-adjoint on $l^2(V)$) if and only if $\deg(G) < \infty$. In this case, $\|\mathbf{A}\| \leqslant \deg(G)$, and $\mathrm{spec}(\mathbf{A}) \subseteq [-\deg(G), \deg(G)]$.*

In [89], also the following basic results are given.

THEOREM 3.2.   *The adjacency operator is compact if and only if G has only finitely many edges.*

THEOREM 3.3.   *If we add or delete finitely many edges in G, then continuous spectrum and eigenvalues of infinite multiplicity remain unchanged.*

THEOREM 3.4.   *Let $G_1, G_2, G_3, \ldots$ be the connected components of G. Then $\operatorname{spec}(\mathbf{A}(G))$ is the closure of $\bigcup \{\operatorname{spec}(\mathbf{A}(G_i)) \mid i = 1, 2, 3, \ldots\}$, and the point spectrum of $\mathbf{A}(G)$ is the union of the point spectra of the $\mathbf{A}(G_i)$.*

Several results concerning spectra of certain products of graphs can be generalized from finite [34] to infinite graphs. As usual, a *simple* graph is assumed to have no multiple edges or loops. Let $G_1, G_2, \ldots, G_n$ be a family of simple graphs, and let B be a nonvoid subset of $\{0, 1\}^n$, not containing the n-tuple $(0, \ldots, 0)$. Then the *non-complete extended p-sum (NEPS) with basis B* of $G_1, \ldots, G_n$ is the graph H with vertex set $V(H) = V(G_1) \times \ldots \times V(G_n)$, in which two vertices $(u_1, \ldots, u_n)$, $(v_1, \ldots, v_n)$ are adjacent if and only if there is an n-tuple $b = (b_1, \ldots, b_n)$ in B with the property that $u_i = v_i$ if $b_i = 0$ and u_i is adjacent to v_i in G_i if $b_i = 1$.

In particular, the basis $B = \{(1, 1, \ldots, 1)\}$ gives rise to the *tensor product* and the basis consisting of all n-dimensional unit vectors leads to the *Cartesian product*. For these types of graph products, we have the following result.

THEOREM 3.5 [91].   *Let $G_1, G_2, \ldots, G_n$ be a family of at most countable graphs with bounded vertex degrees with adjacency operators $\mathbf{A}_1, \mathbf{A}_2, \ldots, \mathbf{A}_n$, respectively, and let H be their NEPS with basis B. Then spectrum and point spectrum of the adjacency operator $\mathbf{A}$ of H are given by*

$$\operatorname{spec}(\mathbf{A}) = \left\{ \sum_{b \in B} \lambda_1^{b_1} \cdot \lambda_2^{b_2} \cdots \lambda_n^{b_n} \mid \lambda_i \in \operatorname{spec}(\mathbf{A}_i) \right\}$$

and

$$\operatorname{spec}_p(\mathbf{A}) = \left\{ \sum_{b \in B} \lambda_1^{b_1} \cdot \lambda_2^{b_2} \cdots \lambda_n^{b_n} \mid \lambda_i \in \operatorname{spec}_p(\mathbf{A}_i) \right\}.$$

We now turn our attention to the transition operator. For u in V, denote by $\mathbf{e}_u$ the unit vector in $l^2(V)$ whose u-entry is equal to one, all other entries are zero. Then $\{\mathbf{e}_u \mid u \in V\}$ is a complete orthonormal system for $l^2(V)$, whereas $\{(\deg(u))^{-\frac{1}{2}} \mathbf{e}_u \mid u \in V\}$ plays the same role for $l^2_\#(V)$.

REMARK 3.6.   *(a)* The transition operator is defined and self-adjoint on $l^2_\#(V)$ for any locally finite graph, $\|\mathbf{P}\| \leqslant 1$ and $\operatorname{spec}(\mathbf{P}) \subseteq [-1, 1]$.
    (b) The analogues of Theorems 3.3 and 3.4 hold in the obvious way for $\mathbf{P}$.

However, there is no immediate analogue of Theorem 3.2 for the transition operator.

THEOREM 3.7.   (a) *The operator $\mathbf{P}$ is Hilbert–Schmidt on $l^2_\#(V)$ if and only if*

$$\sum_{[u, v] \in E} \frac{a^2_{u, v}}{\deg(u) \deg(v)} < \infty.$$

(b) *Each of the following two conditions is necessary for the compactness of* **P**.

(i) *For all* j, k *in* $\mathbb{N}$,

$$\sum (a_{u,v}^2 \mid [u,v] \in E, \deg(u) = j, \deg(v) = k) < \infty.$$

(ii) *For any* $\varepsilon > 0$ *and for all but a finite number (depending on* ε*) of* u *in* V,

$$\sum_{v \sim u} \frac{a_{u,v}^2}{\deg(u)\deg(v)} < \varepsilon.$$

Proof. Note that

$$\langle \mathbf{P}\mathbf{e}_u, \mathbf{e}_v \rangle_\# = \langle \mathbf{A}\mathbf{e}_u, \mathbf{e}_v \rangle = a_{u,v}. \tag{3.1}$$

Thus, the sum in (a) is just the square of the Hilbert–Schmidt norm of **P**:

$$|\mathbf{P}|_{HS}^2 = \sum_{u,v} \left\langle \mathbf{P} \frac{\mathbf{e}_u}{\sqrt{\deg(u)}}, \frac{\mathbf{e}_v}{\sqrt{\deg(v)}} \right\rangle_\#^2.$$

To prove (b), assume that **P** is compact on $l_\#^2(V)$. The set $\{\deg(u)^{-\frac{1}{2}}\mathbf{e}_u \mid u \in V\}$ is bounded, and its image must be relatively compact. Assume that $\{u_n\}$ is a sequence in V such that $\deg(u_n)^{-\frac{1}{2}}\mathbf{P}\mathbf{e}_{u_n} \to \mathbf{x}$ in $l_\#^2(V)$. Then, for every $v \in V$,

$$x_v = \left\langle \mathbf{x}, \frac{1}{\sqrt{\deg(v)}}\mathbf{e}_v \right\rangle_\# = \lim \left\langle \frac{1}{\sqrt{\deg(u_n)}}\mathbf{P}\mathbf{e}_{u_n}, \frac{1}{\sqrt{\deg(v)}}\mathbf{e}_v \right\rangle_\# = \lim \frac{a_{u_n,v}}{\sqrt{\deg(u_n)\deg(v)}}.$$

By local finiteness, $x_v = 0$, and (ii) must hold.

Now assume that the sum in (i) is infinite for some pair of integers j, k. Thus there is an infinite sequence $\{[u_n, v_n]\}$ of edges with $\deg(u_n) = j, \deg(v_n) = k$, and

$$\left\| \frac{1}{\sqrt{\deg(u_n)}}\mathbf{P}\mathbf{e}_{u_n} \right\|_\#^2 \geq \frac{a_{u_n,v_n}^2}{jk} \geq \frac{1}{jk},$$

in contradiction with (ii).

In particular, the analogue of Theorem 3.2 holds for the transition operator, when $\deg(G) < \infty$. Adding or deleting finitely many edges changes the inner product, but the underlying $l_\#^2$-space remains the same, and it is easy to see that Theorem 3.3 remains valid for **P**. On the other hand, we do not know a general result about **P** for NEPS of non-regular graphs which parallels Theorem 3.5. The following is easy to see; compare with [95].

THEOREM 3.8. *If* G *is the tensor product of two locally finite graphs* G_1 *and* G_2, *then*

$$\mathrm{spec}\,(\mathbf{P}(G)) = \mathrm{spec}\,(\mathbf{P}(G_1)) \cdot \mathrm{spec}\,(\mathbf{P}(G_2))$$

and

$$\mathrm{spec}_p\,(\mathbf{P}(G)) = \mathrm{spec}_p\,(\mathbf{P}(G_1)) \cdot \mathrm{spec}_p\,(\mathbf{P}(G_2)).$$

Finally, we make some observations concerning the Laplacians; compare with [35, 37]. For each edge in E, choose and fix an arbitrary orientation. We write $u(e)$ for the origin and $v(e)$ for the endpoint of edge e in this orientation. Now we consider the Hilbert space $l^2(E)$ of vectors $\phi = (\phi_e \mid e \in E)$ with the usual inner product

$$\langle \phi, \psi \rangle = \sum_{e \in E} \phi_e \overline{\psi_e} \tag{3.2}$$

(each oriented edge is counted once). We define the *difference* operators
$\mathbf{d}: l^2(V) \to l^2(E)$ and $\mathbf{d}_\#: l^2_\#(V) \to l^2(E)$ by

$$\mathbf{d}\mathbf{x}_e = x_{v(e)} - x_{u(e)} = \mathbf{d}_\# \mathbf{x}_e, \quad \mathbf{x} \text{ in } l^2(V) \text{ or } l^2_\#(V), \text{ respectively.} \tag{3.3}$$

These operators are sometimes referred to as *oriented incidence* or *oriented coboundary*
operators; see, for example, [12]. Here, we assume that $\deg(G) < \infty$ in the first case
and that G is locally finite in the second, as we have $\langle \mathbf{dx}, \mathbf{dx} \rangle \leqslant 2 \sum_{v \in V} \deg(v) |x_v|^2$.
The same holds for $\mathbf{d}_\#$. Hence

$$\|\mathbf{d}\|^2 \leqslant 2 \deg(G) \quad \text{and} \quad \|\mathbf{d}_\#\|^2 \leqslant 2. \tag{3.4}$$

We remark that $\|\mathbf{dx}\|$ (or $\|\mathbf{d}_\# \mathbf{x}\|$) is usually called the *Dirichlet norm* of $\mathbf{x}$; see [54, 122].
One computes the adjoint operators from $l^2(E)$ into $l^2(V)$ or $l^2_\#(V)$, respectively,

$$\mathbf{d}^*\phi_u = \sum_{v(e)=u} \phi_e - \sum_{u(e)=u} \phi_e, \quad \mathbf{d}_\#^*\phi_u = \frac{1}{\deg(u)} \mathbf{d}^*\phi_u \tag{3.5}$$

and obtains

$$\Delta_A = \mathbf{d}^*\mathbf{d}, \quad \Delta_P = \mathbf{d}_\#^*\mathbf{d}_\#. \tag{3.6}$$

These formulas are useful for the description of properties related to the spectral radii
of $\mathbf{A}$ and $\mathbf{P}$; compare with [13, 35, 37, 54, 91, 122]. In particular, the Laplacians are
positive operators, and we shall be interested in the question when the number zero
is contained in their spectrum; see §5.

4. Spectral radius, walk generating functions and spectral measures

In view of Theorems 3.1, 3.4, we assume for the rest of this paper that G is
connected and locally finite. Furthermore, when talking of the adjacency operator
$\mathbf{A}(G)$, we shall implicitly assume that it is bounded on $l^2(V)$, that is, $\deg(G) < \infty$.
(The latter assumption will not be used for the transition operator.)

Let $\mathbf{B} = \mathbf{B}(G)$ be an arbitrary matrix associated with G having the property

$$b_{u,v} > 0 \text{ if } [u,v] \in E \quad \text{and} \quad b_{u,v} = 0 \text{ if } [u,v] \notin E. \tag{4.1}$$

A *walk* from u to v ($u, v \in V$) is a sequence $\pi = [u = u_0, u_1, u_2, \ldots, u_n = v]$ of successively
adjacent vertices. The *length* of π is $|\pi| = n$, and the *weight* of π with respect to the
matrix $\mathbf{B}$ is

$$w(\pi) = w(\pi \mid \mathbf{B}) = b_{u_0, u_1} b_{u_1, u_2} \ldots b_{u_{n-1}, u_n}. \tag{4.2}$$

For the walk $[u]$ of length 0 ($u \in V$), we set $w([u]) = 1$. If Π is a set of walks, then

$$w(\Pi) = \sum_{\pi \in \Pi} w(\pi). \tag{4.3}$$

As G is locally finite, the matrix powers $\mathbf{B}^n$ are well defined for $n \geqslant 1$, its entries are
denoted $b^{(n)}_{u,v}$. We set $\mathbf{B}^0 = \mathbf{I} = \mathbf{I}(G)$. The following is well known.

THEOREM 4.1. $b^{(n)}_{u,v} = w(\Pi_n(u,v) \mid \mathbf{B})$, *where* $\Pi_n(u,v)$ *is the set of all walks of length*
n *from* u *to* v.

COROLLARY 4.2. *For the adjacency matrix of a simple graph,* $a^{(n)}_{u,v}$ *is the number of*
walks of length n *from* u *to* v.

(To obtain the same result for graphs with multiple edges, one has to specify the edges
in the definition of a walk.)

COROLLARY 4.3. $p_{u,v}^{(n)} = w(\Pi_n(u,v) \mid \mathbf{P}) = \Pr[X_{n+k} = v \mid X_k = u]$ (independent of k) is the probability of reaching v from u in n steps.

Now consider for $z \in \mathbb{C}$ and $u, v \in V$ the power series

$$R_{u,v}(z) = R_{u,v}(z \mid \mathbf{B}) = \sum_{n=0}^{\infty} b_{u,v}^{(n)}/z^{n+1} = \frac{1}{z} w\left(\Pi(u,v) \mid \frac{1}{z}\mathbf{B}\right), \qquad (4.4)$$

where $\Pi(u,v)$ is the set of all finite walks from u to v. This series converges and defines an analytic function for $|z| > r$, where

$$r = r(\mathbf{B}) = \limsup_{n \to \infty} (b_{u,v}^{(n)})^{1/n}. \qquad (4.5)$$

As G is connected, r does not depend on the particular choice of $u, v \in V$ [124, 125], [113, §6.1]. The number $r(\mathbf{B})$ is called the *convergence norm* or (in the self-adjoint case) the *spectral radius* of $\mathbf{B}$. By *Pringsheim's* theorem, r is the largest positive singularity of $R_{u,v}(z \mid \mathbf{B})$. Observe that

$$r(\mathbf{A}) \leqslant \deg(G) \quad \text{and} \quad r(\mathbf{P}) \leqslant 1. \qquad (4.6)$$

Note that our r corresponds to the number $1/R$ of [124, 113, 75] and others. Furthermore, we have by [124], [113, §6.1]

$$\begin{aligned} \text{either} \quad & R_{u,v}(r) < \infty \quad \text{for all} \quad u, v \in V \\ \text{or} \quad & R_{u,v}(r) = \infty \quad \text{for all} \quad u, v \in V. \end{aligned} \qquad (4.7)$$

In the first case, G is called $r(\mathbf{B})$-*transient*, in the second case $r(\mathbf{B})$-*recurrent*. With the exception of Cayley graphs of finitely generated groups, it is an open problem to give a condition of 'geometric' type for an infinite graph or even a tree to be $r(\mathbf{A})$- or $r(\mathbf{P})$-recurrent. This would be of great interest; compare with [50, 55]. For a matrix-theoretical criterion, see [125, Crit. III] and compare with Theorem 6.2 below.

One subdivides $r(\mathbf{B})$-recurrence into the $r(\mathbf{B})$-*null* and the $r(\mathbf{B})$-*positive* case [113, 124, 125, 126] according to whether $b_{u,v}^{(n)} r^{-n}$ converges to zero or not (this is independent of the choice of $u, v \in V$). As $\mathbf{B} = \mathbf{A}(G)$ and $\mathbf{B} = \mathbf{P}(G)$ define self-adjoint operators, $r(\mathbf{B})$-positivity holds in these cases exactly when $r(\mathbf{B})$ is in the point spectrum of $\mathbf{B}$ [126, Theorem 2.2; 113, Theorem 6.4]: in this case, the multiplicity of the eigenvalue $r(\mathbf{B})$ is one, and $-r(\mathbf{B})$ is an eigenvalue (of multiplicity one) if and only if G is bipartite.

We remark that a *finite* graph is always $r(\mathbf{B})$-recurrent for any $\mathbf{B}$, and, in particular, $r(\mathbf{P}) = 1$. In general, if G is $r(\mathbf{P})$-recurrent and $r(\mathbf{P}) = 1$ then one says that G, or the SRW, is *recurrent* (in the usual sense); in any other case G is called *transient*. (Thus at the same time, a graph may well be transient and $r(\mathbf{P})$-recurrent for $r(\mathbf{P}) < 1$.) Contrary to $r(\mathbf{P})$-recurrence, usual recurrence has a probabilistic interpretation: G is recurrent if and only if for some (and hence all) $u, v \in V$,

$$\Pr[X_n = u \text{ for infinitely many } n \mid X_0 = v] = 1. \qquad (4.8)$$

There is a variety of useful conditions for recurrence, for example, [36, 39, 50, 51, 82, 101, 122, 134].

If $\|\mathbf{A}\|$ and $\|\mathbf{P}\|_\#$ denote the norms of $\mathbf{A}(G)$ and $\mathbf{P}(G)$, acting as self-adjoint operators on $l^2(V)$ and $l_\#^2(V)$, respectively, then we have the following general result.

THEOREM 4.4 [41, 89, 102]. (a) $\|A\| = r(A)$ *and* $\operatorname{spec}(A(G))$ *is a compact set contained in the real interval* $[-r(A), r(A)]$; *furthermore,* $r(A) \in \operatorname{spec}(A(G))$.

(b) $\|P\|_* = r(P)$ *and* $\operatorname{spec}(P(G))$ *is a compact set contained in the real interval* $[-r(P), r(P)]$; *furthermore,* $r(P) \in \operatorname{spec}(P(G))$.

This justifies calling r the spectral radius of the corresponding matrix. Now denote for B as above

$$R(z) = R(z \mid B) = (R_{u,v}(z \mid B))_{u,v \in V}. \tag{4.9}$$

Then we have for $|z| > r(B)$

$$R(z \mid B) = \sum_{n=0}^{\infty} \frac{1}{z^{n+1}} B^n \quad \text{and} \quad (zI - B) R(z \mid B) = I, \tag{4.10}$$

where $I = I(G)$. Hence we have the following.

THEOREM 4.5. *Let* $B = A(G)$ *or* $B = P(G)$, *acting on* $l^2(V)$ *or* $l^2_*(V)$, *respectively. Then* $R(z \mid B)$ *extends to an analytic matrix function for z in* $\mathbb{C} \setminus \operatorname{spec}(B(G))$ *(that is, all matrix components are analytic functions of z). The extension, still denoted* $R(z \mid B)$, *defines the* resolvent operator $(zI - B)^{-1}$. *In particular, for* $z \in \mathbb{C} \setminus \operatorname{spec}(B(G))$, *the matrix* $R(z \mid B)$ *defines a bounded linear operator on the corresponding* l^2-*space.*

Denote by $q(G)$ the *parity* of G:

$$q(G) = \begin{cases} 2, & \text{if } G \text{ is bipartite,} \\ 1, & \text{otherwise.} \end{cases} \tag{4.11}$$

Furthermore, for $u, v \in V$ let

$$q(u, v) = \begin{cases} 0, & \text{if } q(G) = 1 \text{ or } d(u, v) \text{ is even,} \\ 1, & \text{if } q(G) = 2 \text{ and } d(u, v) \text{ is odd.} \end{cases} \tag{4.12}$$

Here, as usual, $d(u, v)$ is the distance between u and v, that is, the length of a shortest walk from u to v. Remember that G is assumed to be connected, so that the distance is finite.

THEOREM 4.6 [75, 77, 113]. *Let* $B = B(G)$ *have property* (4.1). *Then we have for all* $u, v \in V$:

(a) $\lim (b_{u,v}^{(m)})^{1/m} = r(B)$, *where* $m = q(G) n + q(u, v)$ *and* $n \to \infty$,

(b) $b_{u,v}^{(n)} \leqslant r(B)^n$,

(c) *if* $B = A(G)$ *or* $B = P(G)$ *then* $\lim (b_{u,u}^{(m+2)} / b_{u,u}^{(m)}) = r(B)^2$, *where* $m = q(G) n$ *and* $n \to \infty$.

We also mention the following general result concerning the transition operator of a connected, locally finite graph; see, for example [55].

THEOREM 4.7. $\lim_{n \to \infty} p_{u,v}^{(n)} = 0$ *for some (and hence all)* $u, v \in V$ *if and only if* G *is infinite.*

The (u, v)-entry $W_{u,v}(z)$ of the matrix

$$W(z) = W(z \mid B) = \frac{1}{z} R\left(\frac{1}{z}\right) = (I - zB)^{-1} \tag{4.13}$$

is the *walk generating function*: if $\mathbf{B} = \mathbf{A}(G)$ and G is simple it counts the walks from u to v, and if $\mathbf{B} = \mathbf{P}(G)$, its coefficients are the transition probabilities from u to v in the SRW. By Theorem 4.5, in each of these two cases $\mathbf{W}(z)$ is well defined and bounded as an operator on the corresponding l^2-space, if $z^{-1} \notin \operatorname{spec}(\mathbf{B})$.

Now denote by $C(\operatorname{spec}(\mathbf{B}))$ the space of all continuous real functions on $\operatorname{spec}(\mathbf{B})$, where $\mathbf{B} = \mathbf{A}(G)$ or $\mathbf{B} = \mathbf{P}(G)$ defines a self-adjoint operator on the corresponding l^2-space. If $f \in C(\operatorname{spec}(\mathbf{B}))$ is a polynomial, then we can define the operator $f(\mathbf{B})$ in the obvious way. By approximation, this correspondence can be extended to define $f(\mathbf{B})$ for all $f \in C(\operatorname{spec}(\mathbf{B}))$ (see [41, §X.2]), and there is an operator-valued set function $\mu = \mu^{\mathbf{B}}$, defined on the Borel sets of $\operatorname{spec}(\mathbf{B})$, such that

$$f(\mathbf{B}) = \int_{\operatorname{spec}(\mathbf{B})} f(\lambda)\,\mu(d\lambda) \tag{4.14}$$

for every such f. Usually, μ is called the *resolution of the identity* for $\mathbf{B}$. In particular, if z, or z^{-1} respectively, lies outside $\operatorname{spec}(\mathbf{B})$, then

$$\mathbf{R}(z\,|\,\mathbf{B}) = \int_{\operatorname{spec}(\mathbf{B})} \frac{1}{z-\lambda}\mu(d\lambda) \quad \text{and} \quad \mathbf{W}(z\,|\,\mathbf{B}) = \int_{\operatorname{spec}(\mathbf{B})} \frac{1}{1-z\lambda}\mu(d\lambda). \tag{4.15}$$

We define the *spectral measures*

$$\mu^{\mathbf{A}}_{u,v}(d\lambda) = \langle \mu^{\mathbf{A}}(d\lambda)\,\mathbf{e}_u, \mathbf{e}_v \rangle, \quad \mu^{\mathbf{P}}_{u,v}(d\lambda) = \frac{1}{\deg(u)}\langle \mu^{\mathbf{P}}(d\lambda)\,\mathbf{e}_u, \mathbf{e}_v \rangle_{\#}, \tag{4.16}$$

where $u, v \in V$. Then in each of the two cases $\mathbf{B} = \mathbf{A}$ or $\mathbf{B} = \mathbf{P}$, (4.15) says that $\mu_{u,v}$ is a regular measure on $\operatorname{spec}(\mathbf{B})$ and

$$W_{u,v}(z) = \int_{\operatorname{spec}(\mathbf{B})} \frac{1}{1-z\lambda}\mu_{u,v}(d\lambda). \tag{4.17}$$

The nth moment of $\mu_{u,v}$ is just

$$b^{(n)}_{u,v} = \int_{\operatorname{spec}(\mathbf{B})} \lambda^n \mu_{u,v}(d\lambda). \tag{4.18}$$

If we set $n = 0$, we see that the total mass of $\mu_{u,v}$ is zero if $u \neq v$ and one if $u = v$. In particular, $\mu_{u,u}$ is a probability measure for $u \in V$. The spectral measures can be determined if the walk generating functions are known. By (4.15), $R_{u,v}(z)$ is the *Stieltjes transform* of $\mu_{u,v}$, and the Stieltjes inversion formula can be applied, see [41, Theorem X.6.1]:

$$\mu_{u,v}((-\infty, \lambda)) = \lim_{\delta \to 0+} \lim_{\varepsilon \to 0+} \frac{1}{2\pi i} \int_{-\infty}^{\lambda - \delta} (R_{u,v}(\alpha - i\varepsilon) - R_{u,v}(\alpha + i\varepsilon))\,d\alpha. \tag{4.19}$$

If we are only interested in those values λ_0 where $\mu_{u,v}$ is continuous, then (4.19) can be simplified to

$$\int_{-\infty}^{\lambda_0} \mu_{u,v}(d\lambda) = -\frac{1}{\pi} \lim_{\varepsilon \to 0+} \int_{-\infty}^{\lambda_0} \operatorname{Im}(R_{u,v}(\alpha + i\varepsilon))\,d\alpha \tag{4.20}$$

(see for example [127]).

Identities (4.18) and (4.19) imply the following generalization of the pairing theorem (see [34, Theorem 3.11] for the finite case) for adjacency or transition operator of a connected graph; see also [57].

THEOREM 4.8. *If G is bipartite then $\mu_{u,v}(d\lambda)$ is symmetric with respect to zero for every pair of vertices u, v which are at even distance. Conversely, if $\mu_{u,v}(d\lambda)$ is symmetric with respect to zero for some pair u, v at even distance, then G is bipartite.*

COROLLARY 4.9 [89]. *If G is bipartite then the spectra of $\mathbf{A}(G)$ and of $\mathbf{P}(G)$ are symmetric with respect to zero. For the point spectrum, this includes multiplicities.*

We mention that for the Cartesian product of two graphs, the spectral measures can be determined from those of the factors. The following theorem has no direct analogue for the transition operator, unless the two factors of the Cartesian product are regular.

THEOREM 4.10. *Let G be the Cartesian product of G_1 and G_2, $\mathbf{A} = \mathbf{A}(G)$ and $\mathbf{A}_i = \mathbf{A}(G_i), i = 1, 2$. Then $\mu^{\mathbf{A}}$ is the convolution of $\mu^{\mathbf{A}_1}$ with $\mu^{\mathbf{A}_2}$.*

In other words, if u, v are vertices of $G, u = (u_1, u_2)$ and $v = (v_1, v_2)$ with $u_i, v_i \in V(G_i)$ then

$$\mu_{u,v}^{\mathbf{A}} = \mu_{u_1, v_1}^{\mathbf{A}_1} * \mu_{u_2, v_2}^{\mathbf{A}_2}, \tag{4.21}$$

where $*$ denotes convolution of real measures (with respect to addition).

Besides (4.19), another method which can be used to determine spectral measures is by 'finite approximations'. The following is well known [41, §X.7; 118].

LEMMA 4.11. *Let $\mathbf{B}_n$ be a sequence of operators converging to $\mathbf{B}$ pointwise in the norm of the underlying l^2-space. Let $\mu^{(n)}$ and μ denote the respective resolutions of the identity. Then $\mu^{(n)}((-\infty, \lambda))$ converges to $\mu((-\infty, \lambda))$ for every λ where μ has no jump.*

We say that a sequence of subgraphs G_n converges to G, if each edge of G is contained in all but finitely many of the G_n. Lemma 4.11 implies the following result.

THEOREM 4.12. *Let G_n be a sequence of subgraphs of G converging to G. Then for every pair u, v of vertices, the sequence of spectral measures $\mu_{u,v}^{(n)}$ of $\mathbf{A}(G_n)$ converges to the spectral measure $\mu_{u,v}$ of $\mathbf{A}(G)$ at all points of continuity of $\mu_{u,v}$.*

In order to calculate spectral measures of an infinite graph G, a possible application of this theorem is to take for G_n an increasing sequence of finite induced subgraphs of G. Note that for a finite graph, the spectral measure is easily determined. For every eigenvalue of the adjacency matrix, it has a jump which can be calculated from the corresponding normalized eigenvector(s). Conversely, the result of [83] concerning the eigenvalue distribution of large graphs with few short cycles can be viewed as an approximation of finite graphs to a regular tree (see [57]), and in fact, the limiting distribution given in [83] is just the spectral measure $\mu_{u,u}$ of a regular tree; compare with [11, 18] and §7 below. A result for finite Cayley graphs similar to that of [83] is proved by this method in [81]. More general applications of the method of finite approximations can be found in [57].

In a similar way to Theorem 4.12, the spectral radius of an infinite graph can be obtained by approximation; compare with [113, §7; 89].

THEOREM 4.13. *Let $\mathbf{A}_n = \mathbf{A}(G_n)$, where G_n is a sequence of subgraphs converging to G, and let $\mathbf{A} = \mathbf{A}(G)$. Then $r(\mathbf{A}_n)$ converges to $r(\mathbf{A})$ from below.*

For the transition operators $\mathbf{P}(G_n)$ of a convergent sequence of subgraphs of G, Theorems 4.12 and 4.13 are not true in the above form. Observe that for finite G_n, $r(\mathbf{P}(G_n)) = 1$ always, whereas $r(\mathbf{P})$ may be less than one. However, the following is true.

THEOREM 4.14.   *Let G_n be a sequence of subgraphs converging to G, and let $\mathbf{P}_n$ be the truncation of $\mathbf{P}(G)$ with respect to G_n. Then $r(\mathbf{P}_n)$, defined by (4.5), converges to $r(\mathbf{P})$ from below, and the spectral measures of $\mathbf{P}_n$ with respect to $l^2_{\#}(V)$ converge to the spectral measures of $\mathbf{P}$ at all points of continuity of the latter.*

Observe that the (u, v)-entry of $\mathbf{P}_n$ is $p_{u,v}$ (of $\mathbf{P}$), so that $\mathbf{P}_n$ is not the transition matrix of G_n. In probabilistic terms, the substochastic matrix $\mathbf{P}_n$ defines a truncated random walk on G_n, and at each point of the boundary of G_n with respect to G, there is a nonzero probability that the random walk 'vanishes' at some exterior point.

We mention a result which is also related to finite approximations. If G has unbounded or infinite vertex degrees then

$$\sup \{r(\mathbf{A}(G')) \,|\, G' \text{ a finite induced subgraph of } G\} = \infty.$$

On the other hand, if one takes the infimum of the bottoms of the spectra of finite subgraphs, then one may obtain a finite number. Some results in this direction can be found in [120].

For finite graphs, the *closed walk generating function*

$$C(z) = C(z \,|\, \mathbf{B}) = \text{trace}\,(\mathbf{W}(z)) \tag{4.22}$$

is of great interest. For infinite graphs, it cannot be defined in the same way; compare with [57] for possible extensions in some cases. Note that for a finite graph, $C(z)$ is a constant multiple of $W_{u,u}(z)$ provided that the graph is *walk-regular* for the associated matrix $\mathbf{B}(G)$: this means that $W_{u,u}(z)$ does not depend on vertex u. If an infinite graph is walk-regular, then it is justified to consider $W_{u,u}(z)$ as an equivalent of $C(z)$. This class includes all vertex transitive graphs, and in particular all Cayley graphs of finitely generated groups. We remark that the corresponding spectral measure $\mu_{u,u}$ is usually called *Plancherel measure* in the transitive case; see for example [45] and §7 below. Its importance is in representation theory of groups on one hand and in multiplicity theory on the other, as it gives the approximate distribution of the spectra of large finite subgraphs of G; compare with [57, 83].

Methods of calculation and explicit formulas of walk generating functions, spectral radius and spectral measures will be given in §7 for a variety of cases.

5. Growth and isoperimetric number of a graph

If u is a vertex of G then the *growth function* of G around u is

$$\beta_u(n) = |\{v \in V \,|\, d(u, v) \leqslant n\}|. \tag{5.1}$$

It describes how fast G expands around u. The growth function is related to the transition operator of G in the following way.

THEOREM 5.1 [55].   *Suppose that $d_0 \leqslant \deg(v) \leqslant \deg(G) < \infty$ for all v in V. Then, for all v,*

$$d_0/\deg(G) \leqslant \beta_v(n)\, p_{v,v}^{(2n)}.$$

From Theorem 4.6b we obtain:

COROLLARY 5.2. $\beta_v(n) \geqslant (d_0/\deg(G)) r(\mathbf{P})^{-2n}$.

Thus, if $r(\mathbf{P}) < 1$ then $\beta_v(n)$ grows exponentially fast. If $\beta_v(n) \geqslant c\rho^n$, where $c > 0$ and $\rho > 1$ then we say that G has *exponential growth*. On the other hand, G has *polynomial growth* if $\beta_v(n)$ is bounded above by a polynomial in n; if

$$c_1 n^k \leqslant \beta_v(n) \leqslant c_2 n^k$$

for all $n > 0$, where $c_1, c_2 > 0$, then G is said to have *polynomial growth of (exact) degree k*. In general, the constants c, or c_1 and c_2, respectively, may depend on v, but—due to connectivity—ρ, or k, respectively, do not rely on the choice of v. Furthermore, G has *subexponential growth* if $\lim_{n \to \infty} \beta_u(n)^{1/n} = 1$.

If G is a *regular* graph then by Corollary 5.2 we have

$$\beta_v(n) \geqslant (\deg(G)/r(\mathbf{A}))^{2n}, \tag{5.2}$$

and if G is vertex-transitive then $\beta_v(n) = \beta(n)$ does not depend on $v \in V$. Finally, if G is the Cayley graph of a finitely generated group, then the property of having polynomial growth with a fixed degree, subexponential or exponential growth remains invariant under a change to another Cayley graph (with respect to a different set of generators) of the same group. The growth function has originally been introduced by Milnor [87] for *groups* as a tool to study curvature of Riemannian manifolds. Subsequently, growth of groups has been studied by several authors. We summarize the main results.

THEOREM 5.3.   *Let G be a Cayley graph of a finitely generated group Γ.*

(a) [10, 130] *If Γ has a nilpotent subgroup of finite index then G has polynomial growth of integer degree.*

(b) [59] *If $\beta(n)$ is bounded above by a polynomial in n, then Γ has a nilpotent subgroup of finite index.*

(c) [88, 130] *If Γ is soluble then G has either polynomial or exponential growth.*

(d) [58] *There are many groups with subexponential, nonpolynomial growth.*

(e) *If Γ has a free subgroup on more than one generator, then G has exponential growth.*

Furthermore, if for a *vertex-transitive* graph G, $\beta(n)$ is bounded by a polynomial in n, then G is 'almost' a Cayley graph of a nilpotent group: see [121] for the details; in particular, G must have polynomial growth of integer degree. For further results in a similar spirit to the following theorem, see §6.

THEOREM 5.4 [9].   *If G is a Cayley graph with subexponential growth, then every solution $\mathbf{h} \in l^\infty(V)$ of $\Delta_\mathbf{A}\mathbf{h} = 0$ (which holds if and only if $\Delta_\mathbf{P}\mathbf{h} = 0$) is constant.*

The *isoperimetric* number of a graph is defined as

$$i(G) = \inf_U \frac{|\partial U|}{|U|}, \tag{5.3}$$

where U runs over all finite subsets of V and ∂U is the set of edges having one end in U and the other in $V \backslash U$. The number $i(G)$ is a discrete analogue of the well known

(Cheeger) isoperimetric constant which is used in the theory of Riemannian manifolds; see [22, 23]. Similarly, we define

$$i_p(G) = \inf_U |\partial U|/S(U), \tag{5.4}$$

where (as above) the infimum refers to all finite subsets of V, and $S(U)$ is the sum of the degrees (in G) of the vertices in U. In [91], $i_p(G)$ is called the *transition isoperimetric number* of G. Observe that

$$i(G) = 0 \Leftrightarrow i_p(G) = 0, \quad \text{if } \deg(G) < \infty. \tag{5.5}$$

For finite graphs (where, in the definition corresponding to (5.3), the sets U in the infimum must not cover more than half of V), isoperimetric numbers and their relation with spectra have been studied by [3, 17, 92] and others. For infinite graphs, isoperimetric numbers, or (strong) isoperimetric inequalities have been considered by [13, 35, 37, 54, 91]; see also [51]. (In some of these references, ∂U is defined as the set of *vertices* in U having a neighbour outside of U, which does not make much difference when $\deg(G) < \infty$.) The relation with the spectral radii of $A(G)$ and $P(G)$ is the following.

THEOREM 5.5 [91]. *Let d_0 and $d_1 = \deg(G)$ be the minimal and the maximal vertex degree in G (the latter may be infinite). Then we have:*

(a)
$$\frac{d_1^2(d_0 - r(A))}{d_1^2 - d_1 - (d_0 - r(A))} \leqslant i(G) \leqslant \sqrt{d_1^2 - r(A)^2},$$

(b)
$$\frac{1 - r(P)}{1 - (2 - r(P))/d_1} \leqslant i_p(G) \leqslant \sqrt{1 - r(P)^2}.$$

The two upper bounds are discrete analogues of the so-called Cheeger inequality [23], well known in the theory of Riemannian manifolds. Results preceding those of Theorem 5.5 were proved in [13, 35, 37, 54]. In particular, one has:

COROLLARY 5.6. (a) [54] $i_p(G) = 0$ *if and only if $r(P) = 1$.*
(b) [13, 51] *If $i(G) > 0$ or $i_p(G) > 0$ then G has exponential growth.*

Note that (b) also follows from Corollary 5.2. Thus,

$$0 \in \text{spec}(\Delta_p(G)) \quad \text{if and only if} \quad i_p(G) = 0. \tag{5.6}$$

Groups whose Cayley graph has $i(G) = 0$ are usually called *amenable* and have many interesting properties of functional analytic type [108]. We also remark that there are (Cayley) graphs with exponential growth, but $i(G) = 0$; they arise from soluble groups which are not nilpotent by finite [111]. In [54], the equivalence of $i(G) = 0$ (or $i_p(G) = 0$) with several further properties of functional analytic and probabilistic type is proved (under the assumption that $\deg(G)$ is finite). For more details concerning the connection between isoperimetric numbers and the growth of graphs, see [91]. In [35, 37, 90], infinite cubic planar graphs with minimal degree at least seven are investigated, and lower bounds on their isoperimetric numbers are obtained; further results in this direction can also be found in [90].

To describe isoperimetric properties of graphs with $i(G) = 0$, one may consider the *k-dimensional isoperimetric number*

$$i^{(k)}(G) = \inf_U \frac{|\partial U|}{|U|^{(k-1)/k}},\tag{5.7}$$

defined in the same way as in (5.3). This is exploited to a very large extent in [122, 123] in order to study probabilistic and functional analytic properties of Markov chains, in particular random walks on Cayley graphs of finitely generated groups.

6. *Positive eigenfunctions*

As in the preceding sections, let G be locally finite and connected, and let $\mathbf{B} = \mathbf{B}(G)$ have property (4.1). Furthermore, assume that G is *infinite* and that $0 < r = r(\mathbf{B}) < \infty$ (this is satisfied if $\mathbf{B} = \mathbf{A}(G)$ and $\deg(G) < \infty$, or if $\mathbf{B} = \mathbf{P}(G)$). Then $\mathbf{B}$ can also be considered as an operator on the cone $\mathscr{F}^+(V)$ of nonnegative functions (vectors) $\mathbf{f} = (f_v)_{v \in V}$: the action is defined as in (2.3); $\mathbf{g} = \mathbf{B}\mathbf{f}$ has coordinates $g_u = \sum_{v \in V} b_{u,v} f_v$. Writing $\mathbf{f} \leqslant \mathbf{g}$ for $\mathbf{f}, \mathbf{g} \in \mathscr{F}^+(V)$ means that the inequality holds coordinatewise. Note that we do not use any Hilbert space structure here. The following is a simple consequence of connectedness of G.

LEMMA 6.1 [109]. *If $\mathbf{B}\mathbf{f} \leqslant z\mathbf{f}$ for $\mathbf{f} \in \mathscr{F}^+(V)$ and $z > 0$, and $\mathbf{f}$ is nonzero, then $f_u > 0$ for all $u \in V$.*

Now, one has another characterization of r.

THEOREM 6.2 [109, 125]. *Let $r = r(\mathbf{B})$. Then*

(a) *for real z, the inequality $\mathbf{B}\mathbf{f} \leqslant z\mathbf{f}$ has a nonzero solution $\mathbf{f}$ in $\mathscr{F}^+(V)$ if and only if $z \geqslant r$;*

(b) *if $z > r$, or if $z = r$ and G is r-transient (see (4.7)), then there are infinitely many linearly independent solutions;*

(c) *if $z = r$ and G is r-recurrent, then there is a unique solution (up to constant multiples), and this solution satisfies $\mathbf{B}\mathbf{f} = r\mathbf{f}$.*

Now consider the cone of *z-harmonic functions* (with respect to $\mathbf{B}$) in $\mathscr{F}^+(V)$,

$$\mathscr{H}_z^+ = \{\mathbf{h} \in \mathscr{F}^+(V) \mid \mathbf{B}\mathbf{h} = z\mathbf{h}\}.\tag{6.1}$$

The following result exhibits a contrast to finite graphs.

THEOREM 6.3 [109, 125]. *The cone $\mathscr{H}_z^+$ is nonvoid if and only if $z \geqslant r$.*

If $\mathbf{B} = \mathbf{P}(G)$ and $z = 1$, then $\mathscr{H}_1^+$ consists of all positive functions $\mathbf{h}$ which have the property that at each vertex u, h_u is the average of the values at the neighbours, and

$$\Delta_A \mathbf{h} = \Delta_P \mathbf{h} = 0.\tag{6.2}$$

Such functions (not only if they are positive) are usually called *harmonic functions* on G, without specifying z.

At this point, one may ask for a description of the cone of positive harmonic functions in the sense of (6.2), or more generally, of all positive z-harmonic functions

with respect to **B**. We briefly describe an abstract approach to this question (compare, for example, with [113, §5.5], where only stochastic matrices are considered, but the results carry over to our case). If $z = r$ and G is $r(\mathbf{B})$-recurrent, then there is a unique solution up to constant multiples. Hence, for the rest of this section, we assume that either $z > r$ or that $z = r$ and G is r-transient, in other words,

$$0 < R_{u,v}(z) < \infty \quad \text{for all } u, v \text{ in } V. \tag{6.3}$$

We select a vertex o, a 'root', and define the *Martin kernel*

$$K_{u,v}(z) = R_{u,v}(z)/R_{o,v}(z), \quad u, v \in V. \tag{6.4}$$

Then there is a compactification $\hat{G}_z$ of $V = V(G)$ which is characterized up to homeomorphism by the following three properties.

(I) $\hat{G}_z$ is compact metrizable and contains V as a dense, discrete subset.
(II) The Martin kernel extends to $V \times \hat{G}_z$ continuously in the second variable (the extension is also denoted by $K_{u,.}(z)$).
(III) If $\alpha, \beta \in \hat{G}_z$ and $K_{u,\alpha}(z) = K_{u,\beta}(z)$ for all $u \in V$, then $\alpha = \beta$.

The set of new points $\mathcal{M}_z = \hat{G}_z \setminus V$ is called the *Martin boundary* of G with respect to **B** and z. Its importance lies in the following result; see, for example, [99, 113].

THEOREM 6.4 (Poisson–Martin representation theorem). *For every function* **h** *in* $\mathcal{H}_z^+$, *there is a positive Borel measure* $\nu_{\mathbf{h}}$ *on* $\mathcal{M}_z$, *such that for every vertex* u,

$$h_u = \int_{\mathcal{M}_z} K_{u,\alpha}(z) \, \nu_{\mathbf{h}}(d\alpha).$$

The measure $\nu_{\mathbf{h}}$ is 'almost' unique, but we do not go into the details of these questions; see, for example, [107]. Given the abstract construction, one is interested in a 'visualization' of the Martin boundary $\mathcal{M}_z$ in terms of the graph structure. This is a difficult task. We remark that for 'tree-like' graphs and a reasonable choice of **B**(G) (including adjacency and transition matrix), $\mathcal{M}_z$ coincides with the *space of ends* of G [106], whereas for integer lattices, $\mathcal{M}_z$ is homeomorphic to the unit sphere in the respective dimension for $z > r$, and consists of one point for $z = r$ [38]. For an overview of results on harmonic functions in a graph-theoretical setting, see [107]. There, only the cone $\mathcal{H}_1^+$ for stochastic **B**(G) is considered, but with some care, most results carry over to the general case.

7. Graphs of groups, distance regular graphs and trees

In this section, we give an overview of results concerning particular classes of graphs. Explicit computational results are known only when the graphs under consideration satisfy some type of regularity property: examples are Cayley graphs of finitely generated groups, vertex-transitive graphs, distance-regular graphs, regular, biregular or radial trees, and so on. For Cayley graphs, results are also known when instead of **A**(G) or **P**(G) one considers any matrix **B**(G) with property (4.1) whose entries remain invariant under the group action, so that **B** is in fact a convolution operator. In the sequel, we shall mainly concentrate on the adjacency matrix and give results for l^2-spectra, walk generating functions and spectral measures.

A. *The two way-infinite path*

We identify the two way-infinite path with $\mathbb{Z}$, the integers; the edges are $\{[u, u+1] \mid u \in \mathbb{Z}\}$. The results in this case are 'folklore'; see, for example, [71, 97]. For $G = \mathbb{Z}$,

$$\text{spec}(A) = [-2, 2] \quad \text{and}$$

$$W_{u,v}(z) = \left(\frac{1 - \sqrt{1 - 4z^2}}{2z}\right)^{|u-v|} \cdot \frac{1}{\sqrt{1 - 4z^2}}. \tag{7.1}$$

The Plancherel measure $\mu_{u,u}$ (independent of u) is absolutely continuous,

$$\mu_{u,u}(d\lambda) = \frac{1}{\pi \sqrt{4 - \lambda^2}} \chi_{[-2, 2]}(\lambda) \, d\lambda, \tag{7.2}$$

where χ denotes an indicator function.

B. *Square lattices*

Many details concerning spectral properties of square lattices can be found in [116]. The d-dimensional square lattice (Figure 1) is d times the Cartesian product of $\mathbb{Z}$ with itself. Hence (see Theorems 3.5 and 4.13), for $G = \mathbb{Z}^d$,

$$\text{spec}(A) = [-2d, 2d], \tag{7.3}$$

the Plancherel measure is the d-fold convolution power of the measure of (7.2), and in particular, the closed walk generating function is

$$W_{u,u}(z) = \frac{1}{\pi^d} \int_0^\pi \cdots \int_0^\pi \frac{1}{1 - 2z(\cos\alpha_1 + \ldots + \cos\alpha_d)} \, d\alpha_1 \ldots d\alpha_d; \tag{7.4}$$

compare, for example, with [70, 96, 103]. The analytic behaviour of $W_{u,u}(z)$ near the 'principal' singularity $z = r(A) = 2d$ is as follows; see, for example, [70] for $d = 3$ and [19, Lemma 4] in general:

$$W_{u,u}(z) = \begin{cases} g_d(z)(2d - z)^{(d-2)/2} + h_d(z), & \text{if } d \text{ is odd, and} \\ g_d(z)(2d - z)^{(d-2)/2} \log(2d - z) + h_d(z), & \text{if } d \text{ is even,} \end{cases} \tag{7.5}$$

where g_d and h_d are analytic in a neighbourhood of $z = 2d$, with $g_d(2d) \neq 0$. Further spectral properties of $\mathbb{Z}^d$ are studied in [6]. Note that $\mathbb{Z}^d$ is the most typical example of a Cayley graph with polynomial growth of degree d. Furthermore, $i(\mathbb{Z}^d) = 0$ and $i^{(k)}(\mathbb{Z}^d) > 0$ if and only if $k \leqslant d$: the 'isoperimetric dimension' of $\mathbb{Z}^d$ is d. Finally, we remark that on $\mathbb{Z}^d$, all positive harmonic functions are constant; see, for example, [116].

C. *The hexagonal chain and other lattice-type graphs*

In [57], the method of finite approximations (Theorem 4.11) is applied to obtain the *cumulative* spectral measure (or its distribution function, respectively) for the infinite hexagonal chain; see Figure 3. This is an appropriate mean of the spectral measures $\mu_{u,u}$, where u ranges in the vertex set. See [57] for details.

Other types of lattice-like graphs have also been studied, for example, infinite tubes (Cayley graphs of $\mathbb{Z} \times \mathbb{Z}_n$) [98] and body-centred cubic lattices [69].
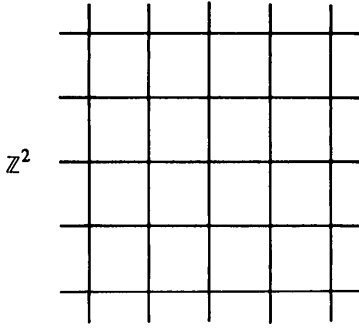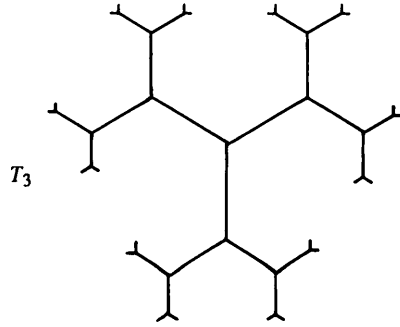
$\mathbb{Z}^2$

FIG. 1

T_3

FIG. 2

FIG. 3

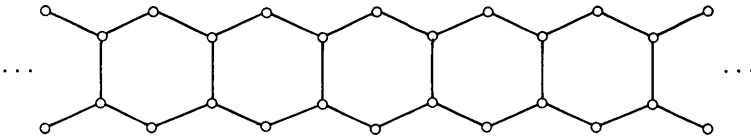### D. Homogeneous trees

Many authors—often independently—have contributed to spectral theory, functional analysis, walk generating functions, random walks, and so on, for the homogeneous (regular) tree T_q of degree q (Figure 2). (Sometimes, the homogeneous tree of degree $q+1$ is indexed with q because of its connection with q-adic groups [114].) If q is even, then T_q is the Cayley graph of a free group, and many papers deal with T_q in this 'disguise'. The 'classical ancestor' is Kesten [76], who (among other things) calculates the closed walk generating function of the transition operator. This appears also in [48, 61], for example. The study of harmonic analysis for the adjacency (or, equivalently, the transition) operator of T_q goes back to [18] and has been developed by many authors. The results are subsumed in the book [45]; we point out the references [11, 24, 25, 27, 40, 44, 83, 110, 112]; further literature can be found in [45]. Some harmonic analysis of T_q can also be found in [81]. For the adjacency operator of T_q we have

$$\mathrm{spec}\,(\mathbf{A}) = [-2\sqrt{q-1}, 2\sqrt{q-1}],$$

$$W_{u,v}(z) = \left(\frac{1-\sqrt{1-4(q-1)z^2}}{2(q-1)z}\right)^{d(u,v)} \cdot \frac{2(q-1)}{(q-2)+q\sqrt{1-4(q-1)z^2}} \quad \text{and} \quad (7.6)$$

$$\mu_{u,u}(d\lambda) = \frac{q\sqrt{4(q-1)-\lambda^2}}{2\pi(q^2-\lambda^2)}\chi_{[-2\sqrt{q-1},\,2\sqrt{q-1}]}(\lambda)\,d\lambda.$$

Considerable attention has also been paid to the l^p-spectrum of $\mathbf{A}(T_q)$ for arbitrary $p \geqslant 1$; see [18, 45, 110]: if $1 \leqslant p < \infty$ and $1/p+1/p' = 1$, then

$$\mathrm{spec}_p(\mathbf{A}) = \{\zeta \in \mathbb{C}\,||\zeta-2\sqrt{q-1}|+|\zeta+2\sqrt{q-1}| \leqslant 2((q-1)^{1/p}+(q-1)^{1/p'})\} \quad (7.7)$$

is an ellipse. Instead of assigning equal weights to each edge, one may also consider arbitrary weights $b_{u,v} > 0, u \sim v$, which remain invariant under the action of the free group or of any group which acts faithfully on T_q. In this case, the walk generating

function is determined implicitly by an algebraic equation [4, 42, 56, 117]. We have

$$r(\mathbf{B}) = \min\{2t + \sum_{v \sim u} (\sqrt{t^2 + b_{u,v} b_{v,u}} - t) \mid t \geqslant 0\}$$

and   (7.8)

$$\|\mathbf{B}\| = \min\{2t + \sum_{v \sim u} (\sqrt{t^2 + (b_{u,v})^2} - t) \mid t \geqslant 0\},$$

where $u \in V(T_q)$ is arbitrary; see [2, 56, 104, 133]. A detailed study of the l^p-spectra and further harmonic analysis for this setting can be found in [117]; see also [4, 5, 7, 46].

E. Distance-regular graphs

A connected graph G is called *distance-regular* if there exists a function $f: \mathbb{N}_0^3 \to \mathbb{N}_0$ such that for all $u, v \in V(G), j, k \in \mathbb{N}_0$,

$$|\{w \in V(G) \mid d(u, w) = j, d(v, w) = k\}| = f(j, k, d(u, v)).$$ (7.9)

The infinite distance-regular graphs have been completely characterized [68]. They are tree-like graphs which can be parametrized by two integer parameters $m, s \geqslant 2$. The distance-regular graph $D_{m,s}$ (denoted $T(m(s-1), s-1)$ in [57]) can be obtained from the semiregular tree $T_{m,s}$ (see subsection G below) in the following way: its vertex set is the bipartite block of degree m, and two vertices constitute an edge if and only if their distance in $T_{m,s}$ is two. Thus, each vertex of $D_{m,s}$ lies in the intersection of exactly m copies of the finite complete graph K_s (see Figure 4), and $D_{m,s}$ is vertex-transitive. In particular, $D_{m,2} = T_m$. The spectral theory of $D_{m,s}$ is similar to that of the homogeneous tree and has been studied in [26, 28, 43, 63, 64, 65, 78, 94]; see also [57]. The walk generating function of its transition operator is calculated in [49]; see also [13].

Writing

$$I_{m,s} = [s - 2 - 2\sqrt{(m-1)(s-1)}, s - 2 + 2\sqrt{(m-1)(s-1)}]$$

and

$$\phi_{m,s}(\lambda) = \frac{m\sqrt{4(m-1)(s-1) - (\lambda - s + 2)^2}}{2\pi(m(s-1) - \lambda)(m + \lambda)},$$ (7.10)

we have for the adjacency operator of $D_{m,s}$:

$$\mathrm{spec}(\mathbf{A}) = \begin{cases} I_{m,s}, & \text{if } m \geqslant s, \\ I_{m,s} \cup \{-m\}, & \text{if } m < s, \end{cases}$$

$$W_{u,u}(z) = \frac{2(m-1)}{(m-2) + m(s-2)z + m\sqrt{(1 - (s-2)z)^2 - 4(m-1)(s-1)z^2}}$$ (7.11)

and

$$\mu_{u,u}(d\lambda) = \begin{cases} \phi_{m,s}(\lambda)\chi_{I_{m,s}}(\lambda)\,d\lambda, & \text{if } m \geqslant s, \\ \phi_{m,s}(\lambda)\chi_{I_{m,s}}(\lambda)\,d\lambda + \dfrac{s-m}{s}\delta_{-m}(\lambda), & \text{if } m < s, \end{cases}$$

where δ_k denotes the unit mass at k.
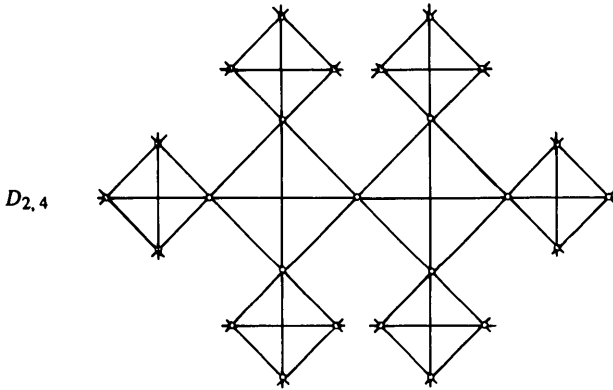
$D_{2,4}$

FIG. 4

F. *Free products*

Let G_1 and G_2 be connected, locally finite graphs which are *vertex-transitive*, each one finite or infinite with at least two vertices. Then we can build up the *free product* $G = G_1 * G_2$ by connecting countably many copies of G_1 and G_2 in the following tree-like way: G is connected, each vertex of G is the intersection of exactly one copy of each of G_1 and G_2, and the only simple circles of G are those occurring in one of the copies of the G_i. Thus, G is also vertex-transitive, and the construction is commutative and associative, so that we can also form the free products $G = G_1 * \ldots * G_m, m \geq 2$. In particular, $D_{m,s}$ is the free product of m copies of K_s. Free products are well known in group theory; if the G_i are Cayley graphs of groups with respect to generating sets A_i, then G is the Cayley graph of the (group-theoretical) free product of these groups with respect to the disjoint union of the A_i.

Besides the cases considered above, the simplest case is that of the free product $G = K_r * K_s$ of two complete graphs with $r > s \geq 2$. The walk generating function of these graphs can be calculated explicitly (by the use of an equitable partition; compare with subsection H below). See [131] for this and further properties of the transition operator, see also [62]. The harmonic analysis of $K_r * K_s$ has been studied in detail in [21]; we refer to these three references for the relevant formulas. The spectral theory of the free product $G = C_r * C_s$ of two *cycles* of length r and s (or of even more cycles) is more complicated and has been studied in some detail in [8].

In the sequel, several authors have independently found a useful formula which allows to calculate the resolvent of a free product of two (or more, even infinitely many) vertex-transitive graphs in terms of an implicit equation arising from the resolvents of the factors [21, 84, 115, 135]. The spectral radius can also be obtained by this means [135]. In all these references, the results are stated in terms of groups and transition operators. We give an outline for the adjacency operator on the free product of two vertex-transitive graphs.

For an arbitrary vertex-transitive graph G, write $W(z) = W_{u,u}(z)$ for the generating function of the closed walks at $u \in V$ with respect to the adjacency matrix. The radius of convergence of this power series is $1/r$, where $r = r(\mathbf{A})$. Let

$$\theta = W(1/r)/r \quad (0 < \theta \leq \infty).$$

LEMMA 7.1 [21, 135].   *There is a function $\Phi(t)$, analytic in an open set containing the real interval $[0, \theta)$, such that*

$$W(z) = \Phi(zW(z))$$

for every complex z in an open set containing the interval $[0, 1/r)$. On $[0, 1/r)$, $\Phi(t)$ is real, strictly increasing and strictly convex.

Now consider two vertex-transitive graphs G_1, G_2 and their free product $G = G_1 * G_2$, with corresponding functions and quantities

$$W_i(z), \ r_i = r(\mathbf{A}(G_i)), \ \theta_i, \ \Phi_i(t) \ (i = 1, 2) \ \text{and} \ W(z), \ r = (\mathbf{A}(G)), \ \theta, \ \Phi(t),$$

respectively. We have the following theorem.

THEOREM 7.2 [21, 84, 115, 135].   *If $\bar{\theta} = \min\{\theta_1, \theta_2\}$ then $\theta \leqslant \bar{\theta}$, $\Phi(t)$ extends analytically to an open set containing the interval $[0, \bar{\theta})$, and in this region,*

$$\Phi(t) = \Phi_1(t) + \Phi_2(t) - 1.$$

Thus, if one knows $W_i(z)$, then $\Phi_i(t)$, can be calculated for $i = 1, 2$, and the implicit equation of Lemma 7.1 which determines $W(z)$ can be found. If $\theta < \bar{\theta}$, then Theorem 7.2 can be used to obtain the asymptotic behaviour of $a_{u,u}^{(n)}$; see [135]:

$$a_{u,u}^{(n)} \sim Cr^n n^{-\frac{3}{2}} \quad \text{as } n \to \infty, \tag{7.12}$$

where $C > 0$. (In case G is bipartite, one has to restrict to even n in (7.12).) This holds, in particular, when $G = G_1 * G_2$, where we do not have $G_1 = G_2 = K_2$, and the vertex-transitive graphs G_1, G_2 are finite or have polynomial growth of degree at most 4 (by combining results of [59, 121, 123, 135]).

G. *Biregular, multiregular and other trees*

The *biregular tree* $T_{k,l}(k, l \geqslant 2)$ is an infinite tree where the vertex degree is constant on each of the two bipartite classes, with values k and l, respectively. If we replace its edge set by new edges which connect every pair of vertices at distance two in the tree, then we obtain two disjoint copies of $D_{k,l}$ and $D_{l,k}$. Thus, the spectral theory of $T_{k,l}$ can be deduced from that of the distance regular graphs (and vice versa), see [57]. An additional reference is [62].

Similarly, we can define the *multiregular tree* $T_{k:l_1,\dots,l_k}(k, l_i \geqslant 2$; see Figure 5): in one of the two bipartite classes, denoted B_1 here, the vertex degree has constant value k. In the other class, the degrees are as follows: each vertex of B_1 has exactly one neighbour of degree $l_i, i = 1, \dots, k$; multiple occurrences of the same value of l_i are taken into account. Thus, $T_{k,l} = T_{k:l_1,\dots,l_k}$ with $l_1 = \dots = l_k = l$. If we add new edges on B_1 by joining all vertices at distance two, then we obtain the free product $K_{l_1} * \dots * K_{l_k}$: we could also say that $T_{k:l_1,\dots,l_k}$ is the 'barycentric subdivision' of the latter graph. This fact is exploited in [105] to study the walk generating function of the transition operator of $T_{k:l_1,\dots,l_k}$, or of the free product, respectively, and to compute the spectral radius, which is given by a formula similar to (7.8). For some other classes of trees, computational results are also available: for example, 'radial' trees (see [51, 132] and subsection H below), and natural spanning trees of $\mathbb{Z}^d$ [52]. In general, it is rather easy to see [53] that an infinite tree T with $\deg(T) < \infty$ has
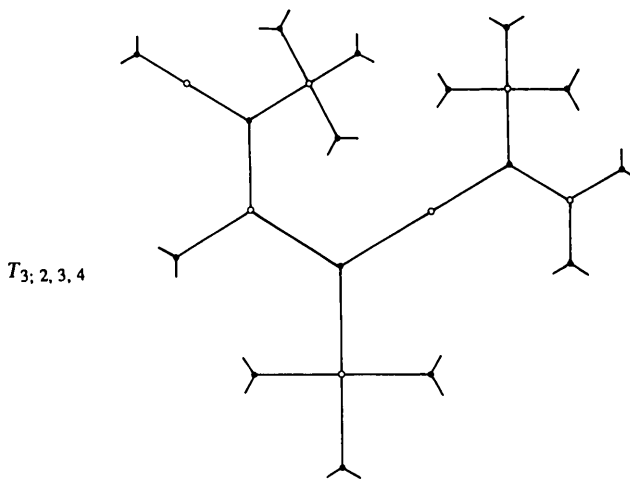
$T_{3;\,2,\,3,\,4}$

FIG. 5

isoperimetric number $i(T) > 0$ (recall that this is equivalent with $r(\mathbf{P}(T)) < 1$) if and only if there is an upper bound on the size of those induced subgraphs which are paths.

H. The use of equitable partitions

Consider a matrix $\mathbf{B}(G)$ which satisfies (4.1) and a partition of $V(G)$ into finite sets $V_i, i \in I$, where the index set is $\mathbb{N}_0$ or $\mathbb{Z}$ (or some other countable set). It gives rise to an *equitable* partition (or a *front divisor*) if the following condition is satisfied: for all $i, j \in I$, the numbers

$$d_{i,j} = \sum_{v \in V_j} b_{u,v} \tag{7.13}$$

are independent of the choice of u in V_i.

We can then form the matrix $\mathbf{D} = (d_{i,j})_{i,j \in I}$, and hope that it is easier to handle than $\mathbf{B}(G)$: in [94], the relation between the spectra of $A(G)$ and of $\mathbf{D}$ (with an appropriate normalization) is studied and applied to distance regular graphs. Equitable partitions have also been used in [49, 50, 131, 132]. The method is particularly rewarding when $\mathbf{D}$ is compatible in the sense of (4.1) with the structure of $\mathbb{N}_0$ or $\mathbb{Z}$, the one or two way-infinite path with or without loops. Very often, one can choose a reference vertex o and use the *distance partition*:

$$V_i = \{v \in V(G) \mid d(v, o) = i\}, i \geqslant 0.$$

If it is equitable, then we have for the closed walk generating function at o that

$$W_{o,o}(z \mid \mathbf{B}) = W_{o,o}(z \mid \mathbf{D}), \tag{7.14}$$

and the latter may be computed as a *continued fraction*

$$W_{o,o}(z \mid \mathbf{D}) = \cfrac{1}{\left|1 - d_{0,0}z\right.} - \cfrac{d_{0,1}d_{1,0}z^2\left.\right|}{\left|1 - d_{1,1}z\right.} - \cdots - \cfrac{d_{i-1,i}d_{i,i-1}z^2\left.\right|}{\left|1 - d_{i,i}z\right.} - \cdots. \tag{7.15}$$

For analytic continued fractions, a well developed theory is available; see, for example, [127]. In [50, 132] this is exploited to study walk generating functions

of *radial trees*, that is, trees whose adjacency matrix is equitable for the distance partition with respect to some reference vertex. Furthermore, the computation of the spectral measure $\mu_{o,o}(d\lambda)$ also becomes an easier task. Compare with [71]; see also [73, 74].

8. *Some remarks on applications in chemistry and physics*

Graphs and their spectra often appear in the applied physical sciences. Some applications are described in [34, Chapter 8]. The adjacency operator appears, for example, in Hückel's theory [86] (discrete approximations of the Schrödinger equation). We point out some early references: [14, 15, 16, 31, 79]. The difference Laplacian is the matrix of a quadratic form expressing the energy of a discrete system. It naturally describes the vibration of a membrane [29, 47], or thermodynamic properties of crystalline lattices [85]. The graphs under consideration are not always infinite, but often refining the discrete approximation means passing to an infinite graph in the limit. This allows, for example, the use of Theorems 4.12 and 4.13.

On the other hand, there is an enormous amount of literature in various scientific areas concerning random walks, in particular the transition operator on finite and infinite graphs and its applications. Of course, the point of view does not always concern spectral aspects. We mention the two surveys [60, 128] and the bibliography [80], and we point out a few papers: [66, 67, 69, 70, 96, 97, 98] for infinite lattice-type graphs and [61, 62, 72, 112] for trees and free products.

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NOTE ADDED IN PROOF. We give some further references which were brought to our attention after submitting this survey [136–142].

In [137], the harmonic analysis of biregular trees is studied in detail, and in [136] some light is shed on the phenomenon of the point spectrum in this case; compare with §7, subsection G and (7.10). In [138] it is shown that for a vertex-transitive graph G, $r(\mathbf{P}) = 1$ ($\Leftrightarrow r(\mathbf{A}) = \deg(G)$) if and only if the automorphism group is amenable and unimodular as a topological group. This is applied to show that $r(\mathbf{P}) < 1$ and $i(G) > 0$ for every vertex-transitive graph with infinitely many ends.

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