QUANTUM STAR GRAPHS AND RELATED SYSTEMS

By

Gregory Berkolaiko

School of Mathematics

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Author's Declaration

I declare that the work in this thesis was carried out in accordance with the Regulations of the University of Bristol. The work is original except where indicated by special reference in the text and no part of the dissertation has been submitted for any other degree. Any views expressed in the dissertation are those of the author and in no way represent those of the University of Bristol. The thesis has not been presented to any other University for examination either in the United Kingdom or overseas.

Gregory Berkolaiko

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Abstract

We calculate the two-point spectral statistics for a class of quantum graphs in the limit as the number of vertices tends to infinity. This is done two ways. The first way uses the exact trace formula and a classification of the periodic orbits on the graph. The second involves a direct study of the statistics of the zeros of a transcendental eigenvalue equation. We show that these approaches produce equivalent results. The first expression we derive takes the form of a power series and is more efficient for numerical computations, while the second involves an improper integral and is in a convenient form to study the singularities of the form factor (the Fourier transform of the two-point correlation function). We also find that the spectral statistics are the same as those already found for the Šeba billiard and we discuss the reasons for this coincidence. As an application of the combinatorial methods developed in this work we derive an exact expression for the quantum return probability on infinite regular trees and analyse it numerically. We conclude that, for certain values a parameter, the return probability tends to a non-zero limit, and, as a consequence, that there exist localised eigenstates.

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Contents

Chapter 1

Introduction

When studying a large class of systems exhibiting a certain property, it usually helps to consider, as an example, a smaller subclass of simpler systems. Then, after finding out how the property arises in the simpler systems, one can hopefully gain some insight into what is happening in the general case.

This "class — subclass" relation is the connection between the quantum chaos and quantum graphs and, to a lesser extent, between quantum graphs and quantum star graphs.

So what is quantum chaos? Naturally, it is the subject studied by quantum chaology,

> the study of semiclassical, but non-classical, behaviour characteristic of systems whose classical motion exhibits chaos. 'Semiclassical' here means 'as Planck's constant tends to zero' [1].

The present work is related to a part of quantum chaology, the study of the eigenvalues of the quantum systems, their *spectrum*. The spectra, although different from system to system, have some universal features which are stated in the conjectures:

Conjecture 1 (Berry-Tabor Conjecture). *If the classical dynamics is integrable then the statistical properties of the spectrum are generically the same*

as those of an uncorrelated sequence of levels, in particular the nearest neighbour spacings distribution is Poissonian [2].

Conjecture 2 (Bohigas-Giannoni-Schmit Conjecture). *If the classical motion of a quantum system is chaotic then the statistical properties of the spectrum are generically the same as those of eigenvalues of a large random matrix from the Gaussian Orthogonal Ensemble (GOE) if the system is invariant under time reversal and from the Gaussian Unitary Ensemble (GUE) if it is not [3].*

By the statistical properties we understand the functions such as the distribution of the spacing between neighbouring eigenvalues, various correlation functions of the sequence of the eigenvalues and associated functions. The Gaussian Orthogonal (Unitary) Ensemble is defined as the probability space of real symmetric (Hermitian) matrices with the statistically independent matrix elements endowed with the probability measure which is invariant under any orthogonal (unitary) change of basis. The study of the statistical properties of such random matrices is a part of Random Matrix Theory (RMT).

The above conjectures do not hold for all systems, there are known counterexamples to Berry-Tabor Conjecture (a good review of the cases in which the Conjecture can be proved or disproved rigorously is given in [4]), and to Bohigas-Giannoni-Schmit Conjecture, e.g. the geodesic motion on certain arithmetic surfaces of constant negative curvature [5], and the cat maps [6]. The conjectures are expected to hold for *generic* systems where the meaning of the word "generic" is the big open question of the field.

There are several approaches which allow one to study the statistical properties of the eigenlevels. For example, the level dynamics, which is the study of the dependence of the eigenlevels on a parameter, makes it possible to trace the transitions from one type of statistical behaviour to another (for instance, the transition from GOE to GUE when the time-reversal symmetry is being broken). In this work, however, we will be mostly concerned with the approach

which originates from the following observation.

For the conjectures to hold at all, the quantum system must know about the chaotic (or not) behaviour of its classical counterpart. And the chaos is defined through the properties of the orbits of the system, e.g. one of the requirements is that almost all of the orbits explore the whole of the available space in their wanderings. Thus one can say that the quantum system must know about the orbits of the classical system. This connection is provided by trace formulae.

A trace formula is a relation between the eigenvalues of the quantum system and the *periodic* orbits of the underlying classical system. In general it is an asymptotic formula, the so-called Gutzwiller trace formula [7], but it becomes exact for certain classes of systems, such as systems of constant negative curvature, and then it is referred to as Selberg trace formula [8, 9]. The information about the spectrum is coded in the form of the density function, a function which has δ-peaks at the points of the real line corresponding to the eigenvalues E_n. The periodic orbits provide the coefficients of the decomposition of the density functions into a sum of cosines:

$$d(E) \equiv \sum_{n=1}^{\infty} \delta(E - E_n) \sim \overline{d}(E) + \frac{2}{\hbar^{1+\eta}} \sum_{p} \sum_{k=1}^{\infty} A_{p,k} \cos\left(\frac{k}{\hbar}(S_p + \mu_p)\right). \tag{1.0.1}$$

Here p stands for periodic orbit, S_p is the action of p, $A_{p,k}$ is an amplitude related to the stability of the kth repetition of p, and μ_p is its Maslov index; $\overline{d}(E)$ is the mean density, that is the average number of the eigenvalues E_n per interval of unit length. The parameter η is equal to zero if the system is classically chaotic and $\eta = (n-1)/2$ if the system is integrable with n degrees of freedom.

It is widely believed that the trace formula contains all the information needed to verify the conjecture but extracting this information is an extremely difficult task. The contributions from different orbits balance very finely and there are a lot of orbits to account for: their number increases exponentially

with the length of the orbits. It turns out, however, that it is possible to extract some information about the density of the periodic orbits weighted with $A_{p,k}^2$ without having the detailed knowledge about the periodic orbits of the system. An important step in this direction was made by Hannay and Ozorio de Almeida [10] who discovered that

$$\sum_{p\,:\,|S_p|<S} A_p^2 \;\sim\; \begin{cases} \alpha S & \text{integrable,} \\ \beta S^2 & \text{chaotic (ergodic),} \end{cases} \tag{1.0.2}$$

as $S \to \infty$. As we see, there is a clear distinction between the asymptotic behaviour of the sum in the integrable and chaotic cases. The Hannay-Ozorio de Almeida sum rule was used by Berry in [11] where, among other quantities, Berry considered the form factor which is the Fourier transform of the spectral two-point correlation function

$$R_2(x) = \langle d(E)d(E+x)\rangle, \tag{1.0.3}$$

where $\langle\,\cdot\,\rangle$ denotes an energy average (there are also other types of averages, and an average with respect to an ensemble of systems will be employed by us later). Using the Gutzwiller trace formula one can obtain an approximation to $R_2(x)$ in the form of a sum over all pairs of periodic orbits. Applying the Fourier transform

$$K(\tau) = \int_{-\infty}^{\infty} R_2(x) e^{ix\tau/\hbar} dx, \tag{1.0.4}$$

one obtains an expression for the form factor $K(\tau)$ as a sum over pairs of orbits too. Berry's analysis was based mostly on the diagonal approximation which means that only the pairs of orbits which are identical with respect to the system's symmetries are kept. However the validity of the approximation is restricted to the range $\tau \ll 2\pi\hbar\overline{d}$ and the calculation outside this range necessarily involves evaluation of the off-diagonal terms associated with the pairs of the orbits not related by symmetry.

The off-diagonal terms are connected with the correlations between the actions of different orbits and in [12] it was shown that one can "reverse" the

Bohigas-Giannoni-Schmit Conjecture: assuming that the spectral fluctuation follow RMT, a universal expression for the classical action correlation function was derived, supported by some numerical evidence. But the breakthrough came from a slightly different direction, or rather from two directions at the same time. The leading order oscillatory term in the RMT-predicted $R_2(x)$ was recovered in [13] using supersymmetry approach (an accessible explanation of the supersymmetry technique is contained, for example, in [14]) and in [15] by relating the off-diagonal terms in the periodic orbit expansion to the diagonal ones. Still the underlying assumption in [15] was, roughly speaking, that the correlations between short periodic orbits cancel each other. The understanding of how it happens (and when it does not, why not) could not only provide a base for the above assumption but to show the way to recover the higher order terms too. To gain some intuition into such balancing between the off-diagonal terms, it was necessary to find an easy example where the periodic orbits and their correlations could be studied in detail.

Enter the quantum graphs. The idea was to consider the eigenvalues of a Laplacian on a metric graph. A graph is a collection of vertices and bonds which connect some of the vertices. A graph becomes metric if we specify the lengths of the bonds. Except at the vertices, the graph is a one-dimensional structure so the differential equation is easily solvable. The boundary conditions, imposed on the vertices, would make finding eigenvalues a nontrivial but still a manageable task and would hopefully ensure that the RMT effects are present. The idea, it seems, was around for some time: the statistical properties of the spectrum of discrete Laplacian were studied, for instance, in [16] and the exact trace formula, this main ingredient of a relevant example, was proved for continuous Laplacian in [17]. It was independently rediscovered in [19, 20], which sparked a whole series of papers, reviewed below, and research projects, including this work.

The results of numerical simulations reported in [19] showed good agreement with the predictions of the RMT, thus establishing validity of the quan-

tum graphs as a toy model of the quantum chaos. Indeed, the necessary ingredients such as the ergodicity (in the Markov chain sense), the exponential proliferation of the periodic orbits, and the trace formula were present. The phenomenon, the affinity with RMT results, was shown to be there as well. There was a drawback that the quantum graphs did not have deterministic classical counterparts, only the probabilistic ones (Markov chains). But it was an advantage at the same time: it was easier to characterise the orbits.

In the next, more detailed, study of the quantum graphs [20] the setup was extended to include more general boundary conditions now depending on a parameter. It was shown numerically with an analytical justification that for different values of the parameter, the statistics undergo a change from being RMT-like to Poissonian. It was also found that the statistics for star graphs (a particular type of graphs, see Fig. 2.1 in the next Chapter; sometimes it is also called Hydra graphs) show systematic deviations from RMT behaviour. As the name suggests, a star graph consists of a central vertex (the body of the Hydra) connected to many periphery vertices (numerous heads of the Hydra). The deviations in the statistics of star graphs become apparent only for sufficiently large number of the periphery vertices.

In was also found in [20] that the multiply connected rings (another type of graphs) have exponentially localised eigenstates (Anderson localisation). A thorough analytical treatment of the Anderson localisation in terms of the periodic orbits on infinite chain graphs was presented in [21]. The infinite chain graph is a graph composed from an infinite number of sequentially connected vertices. Thus, the valency (the number of bonds commencing from a vertex) of each vertex is 2. The quantity considered was the quantum probability to return to the origin: a specified initial condition was iterated using a quantum evolution operator and then the modulus squared of the resulting state was computed at the origin. The classical counterpart of the quantum return probability is the probability for a random walker to return to the origin after n steps. It is well known that this probability decays with n. It turned out

that the quantum return probability does not decay to zero as the number of iterates n tends to infinity, but saturates at a non-zero value. This effect is a result of the interference between orbits of the same length.

A work in a different direction [22] established that the quantum graphs can also be used to study the generic behaviour of chaotic scattering systems. By connecting vertices of a graph by leads to infinity the graph was turned into a scattering problem. It was shown that such graphs display all features which characterise quantum chaotic scattering and, when considered statistically, the ensemble of scattering matrices reproduced quite well the predictions of appropriately defined Random Matrix ensembles.

In [23] an example of the quantum graph whose spectral two-point correlation function reproduces the corresponding RMT expression exactly was found. The two-point correlation function for 2-star graph (a star with only two rays) was computed both directly and through the periodic orbits approach. Upon suitable averaging over the parameter space the result would reproduce the corresponding RMT expression for 2×2 matrices. To prove the equivalence of two approaches, several new combinatorial identities were derived. These identities were later employed in [21] to derive a compact form of the return probability.

Another statistic, the form factor, was studied in detail for star graphs with large number of rays in [24]. Basing on the periodic orbit theory, the full (including the off-diagonal terms!) power series expansion around zero of the form factor was obtained. Remarkably, the first four terms of the expansion were the same as those in the diagonal approximation derived in [20], but the higher terms did not agree. The series obtained in [24], on its interval of convergence, perfectly fitted the numerical data of [20], which was not RMT but in certain sense an intermediate between RMT and Poisson. The radius of convergence of the series was later extended using Padé method of improving convergence. The results of the paper [24] constitute the major part of Chapter 3.

The form factor was also studied in [25], where the periodic orbits expansions were used to compute it explicitly for several directed binary graphs. The results showed good agreement with the RMT and promised to show an even better one if the graph size was increased. Unfortunately certain features in the larger binary graphs made the application of exact combinatorial methods developed in [25] impossible. Still, one of the important contributions of [25] was to find a simpler class of graphs which exhibit RMT effects.

In the papers mentioned above different types of averaging were applied to the spectral statistics of the quantum graphs. The current work employs, in different Chapters, spectrum averaging and averaging with respect to the individual lengths of the bonds. Averaging over the boundary conditions is also possible and in [26] it was demonstrated that these types of averaging are equivalent.

Quantum graphs also attracted a lot of attention recently in connection with the transport and thermodynamic properties of weakly disordered and coherent conductors. These properties can be related to the spectral determinant of the Laplacian on a graph [27]. The various expression for the spectral determinant were studied in detail and an easy-to-use diagrammatic method of expansion of the spectral determinant in terms of a finite number of periodic orbits was derived in [28] (see also references therein).

A method to derive the level spacing distribution $P(\Delta)$ for the quantum graphs without resorting to the periodic orbit theory was presented in [29]. The authors express the eigenvalues of the system as the times at which a hypersurface, explicitly defined by the topology of the graph, is intersected by an ergodic flow on a torus. The level spacings are then explicitly related to the time of first return to the hypersurface. An exact representation of the level spacing distribution is obtained in the form of an integral over the hypersurface. The small Δ behaviour comes from the near the singularities of the hypersurface and can be studied using an approximation of the hypersurface near the singularities. The analysis is performed for several simple graphs,

including the star graph with 3 bonds for which the RMT-like level repulsion is observed for small Δ.

In the present work we try to advance the understanding of the "constructive interference" of the periodic orbits which produces particular statistics. In Chapter 2 we give the definitions of the graphs and periodic orbits, define the Laplacian and the boundary conditions. It is possible to write an explicit solution of the Laplacian and we obtain the eigenvalue condition in the form of a determinant equation. Then we present a simple derivation of the trace formula for the quantum graphs. Having the trace formula at hand we move on to define the spectral statistics, such as the average (mean) density of the eigenvalues, the two-point correlation function and the form factor. We express the latter two statistics as sums over pairs of periodic orbits and show that only the pairs of orbits of the same lengths contribute to the sums. Note that the equality of the lengths of orbits p and p' does not necessarily imply that the orbits are the same or related through some symmetry (e.g. reversing the direction of the orbit). The length of an orbit is simply the sum of lengths of all the bonds it passes, therefore, in order to have the same lengths, two orbits must pass through the same bonds the same number of times (although in a different order), or, using the terminology introduced in [25], have the same bond staying rates. This subject is discussed in detail and illustrated with examples in Chapter 2.

The next Chapter, largely based on the material of [24], is devoted to the detailed study of the star graphs. Here we assume the Neumann boundary conditions and derive a power series expansion of the form factor in the limit as the number of bonds (rays) of the star tends to infinity. To do so we derive an exact combinatorial expression for the form factor for any finite number of bonds and then take the limit which simplifies the combinatorial sums. The expression we obtain, however, is still too complicated to be studied analytically so we compute exactly a large number of terms and then study

them numerically. In particular we find that the radius of convergence of the series is finite and that one can extend the convergence by applying the Padé approximation. Padé approximation to the form factor seems to capture singularities lying in the complex plane and, judging by the character of the approximation, the singularities are not poles but essential singularities.

It turns out that the combinatorial methods developed in Chapter 3 can be applied to study the Anderson localisation on infinite regular trees (also called Bethe lattices in the literature). A graph is a tree if there are no cycles on it and it is regular if the valency of all vertices is the same. The infinite line is a special case of the infinite regular trees corresponding to the valency 2. The Anderson localisation in a similar model (but not identical) was already studied in [31] using the connection between the localisation of the eigenstates and the probability distribution of $\partial\Psi(E)/\partial E$, where the equation

$$\Psi(E) = 2\pi l \tag{1.0.5}$$

is satisfied by the eigenvalues E_n. It was found that there are four ranges in the parameter space where different types of eigenstates exist. In particular, there is a range where the system has normalizable eigenstates and, therefore, there is a pure point component in the spectrum. In Chapter 4 we approach the problem from a different viewpoint. We study the quantum probability to return to the origin of the tree after n steps. Bringing together the methods developed in [21] and [24], we derive an exact combinatorial recursion for the return probability. Again, it is too complicated to be solved analytically but it gives a clear algorithm to analyse the problem numerically. Our algorithm is of polynomial complexity as opposed to exponential complexity if one is to explicitly count all periodic orbits. Our numerical simulations show that for a certain range of the parameter values the return probability tends to a non-zero limit as the number of steps goes to infinity. This implies existence of localised eigenstates. Our result agrees with those presented in [31], even the ranges are in approximate agreement.

In Chapter 5 we return to the star graphs but using a different approach. As explained in Chapter 2, the condition for E_n to be an eigenvalue is that a certain determinant is equal to zero. This determinant takes a particularly simple form for the star graphs, due to their special structure. Then the eigenvalues of the Laplacian are the zeros of a quasi-periodic meromorphic function. We apply the technique developed in [32] to derive the two-point correlation function of the zeros. The two-point correlation function is related to the form factor of Chapter 3 through the Fourier transform and we show that it is indeed the case, that is the answers derived by two completely different approaches are the same. It provides us with another confirmation of the fact that the summation over the periodic orbits is possible and gives the right answer, although it might be difficult to perform.

Chapter 5 gives us a representation of the form factor in the form of an integral. This integral contains all the information about the form factor, in particular the information about the singularities. Studying the integral we find the particular pair of the singularities which caused the divergence of the series of Chapter 3. As concluded earlier from the Padé analysis, the singularities are not poles, in fact we find that they are logarithmic. We calculate the dominant contribution at the singularities and as a corollary obtain the asymptotics of the coefficients of the power series expansion of the form factor. We also notice that the resulting expression for the two-point correlation function is exactly the same as the expression obtained in [32] for the two-point correlation of the spectrum of the Šeba billiard [33, 34], an integrable system perturbed by a delta-function. Heuristically, the reason for such affinity is that the wave dynamics in both systems is centred around the point scatterer, the delta function in the billiard and the central vertex in the star graphs.

The "heavy" combinatorial derivations used in the text are deferred to the Appendix. The derivation of the number of permutations without liaisons, a combinatorial quantity used in Chapters 3 and 4, was significantly simplified

from its original form [24]. The derivations are illustrated with several figures so if the reader chooses to enter the Appendix he should not abandon all hope.

To summarise, we present a derivation of the two-point spectral statistics for a class of quantum graphs in the limit as number of vertices tends to infinity. We derive it in two ways. The first way uses the exact trace formula and a classification of the periodic orbits on the graph; to the best of our knowledge it is the first exact derivation of its kind. The second way studies the statistics of the zeros of the transcendental eigenvalue equation directly. We show that these approaches produce equivalent results which complement each other: the first result obtained in the form of the power series expansion is more efficient for numerical computations and the second result is in a convenient form to study the singularities of the statistic. We also find that the spectral statistics are the same as those already found for Šeba billiard and we discuss the reasons for this coincidence. As an application of the combinatorial methods developed in the work we derive an exact expression for the quantum return probability on the infinite regular trees and analyse it numerically. We conclude that for a certain range of the parameter values the return probability tends to a non-zero limit, hence there are localised eigenstates.

Chapter 2

Definitions and preliminaries

2.1 Definitions

Let $G = (\mathcal{V}, \mathcal{B})$ be a graph where $\mathcal{V}$ is a finite set of vertices and $\mathcal{B}$ is the set of bonds,

$$\mathcal{B} \subset \mathcal{V} \times \mathcal{V} \tag{2.1.1}$$

The set $\mathcal{B}$ is symmetric in the sense that $b = (i, j) \in \mathcal{B}$ iff $\overline{b} = (j, i) \in \mathcal{B}$, where $i, j \in \mathcal{V}$. We only consider graphs without loops, that is $(j, j) \notin \mathcal{B}$. The bonds $b = (i, j)$, as we defined them, are directed: they have an initial vertex, the vertex i, and an end-vertex, the vertex j; $\overline{b}$ denotes the reversal of the bond b. When we refer to "the non-directed bond (i, j)", we mean the couple of bonds, (i, j) and $\overline{(i, j)} = (j, i)$. The number of vertices is denoted by $V = |\mathcal{V}|$ and the number of directed bonds is $2B = |\mathcal{B}|$. The vertices are usually marked by the integers starting from 0 thus the set $\mathcal{V} = (0, \ldots, V - 1)$.

Definition 1. Associated to every graph is its $V \times V$ *connectivity (adjacency) matrix* $\mathbf{C}$. Its elements are given by

$$C_{i,j} = \begin{cases} 1 \text{ if } (i, j) \in \mathcal{B} \\ 0 \text{ otherwise} \end{cases}, \qquad i, j = 1, ..., V. \tag{2.1.2}$$

Since the set $\mathcal{B}$ is symmetric, the matrix $\mathbf{C}$ is symmetric too.

Definition 2. The *valency* v_i of the vertex i is the number of vertices j which are connected to i, i.e.

$$v_i = \sum_j C_{i,j}. \tag{2.1.3}$$

Definition 3. The *bond connectivity matrix* is the $2B \times 2B$ matrix $\mathbf{B}$ with the elements

$$B_{(i,j)(k,l)} = \delta_{jk}, \tag{2.1.4}$$

where (i,j), $(k,l) \in \mathcal{B}$.

Example 1. The *complete graph* K^V is the graph with $\mathcal{V} = \{1, \dots, V\}$ and $\mathcal{B} = \mathcal{V} \times \mathcal{V}$. That is there is a bond (i,j) for any i and j from $\mathcal{V}$. The connectivity matrix of such a graph has zeros on the diagonal and ones as its off-diagonal elements. The valency is the same for each vertex, it is equal to $V-1$.

Definition 4. A sequence of bonds $\{b_i\}_{i=1}^n$, such that $B_{b_i,b_{i+1}} = 1$ for all i, is called a *cycle* if $B_{b_n,b_1} = 1$ and $b_i \neq b_j$, $b_i \neq \overline{b_j}$ for all $i \neq j$.

Example 2. The *tree* is any connected graph with $V = B + 1$. The prime property of a tree is the absence of cycles.

Example 3. The *star graph* (also called Hydra graph) is a tree with $\mathcal{V} = \{0, 1, \dots, B\}$ and the set of edges $\mathcal{B} = \{(0,i),\ (i,0) \colon i = 1, \dots, B\}$. The valency of each vertex is equal to 1 except for the vertex 0 with the valency B.

Let $\widetilde{\mathcal{P}}_n$ be the set of all sequences

$$\mathbf{p} = [b_1, b_2, \dots, b_n], \qquad b_i \in \mathcal{B}, \qquad n \geq 2 \tag{2.1.5}$$

compatible with $\mathbf{B}$ in the sense that $B_{b_i b_{i+1}} = 1$ for $i = 1, \dots, n$ where by b_{n+1} we understand b_1. We denote by $\widetilde{\mathcal{P}}$ the union of all $\widetilde{\mathcal{P}}_n$,

$$\widetilde{\mathcal{P}} = \bigcup_{n=2}^{\infty} \widetilde{\mathcal{P}}_n, \tag{2.1.6}$$

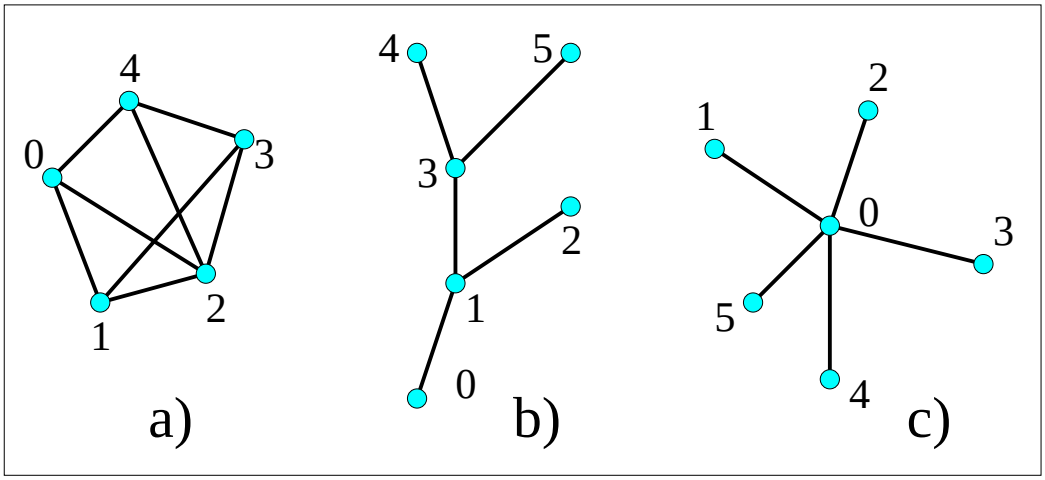

Figure 2.1: Examples of a graph (a), a tree (b) and a star graph (c).

(since there are no loops, $\widetilde{\mathcal{P}}_1 = \emptyset$). Define the cyclic shift operator σ on $\widetilde{\mathcal{P}}_n$ by

$$\sigma\Big([b_1, b_2, \dots, b_n]\Big) = [b_2, b_3, \dots, b_n, b_1]. \tag{2.1.7}$$

We denote by $\mathcal{P}_n = \widetilde{\mathcal{P}}_n/\sigma$ the set of all equivalence classes in $\widetilde{\mathcal{P}}_n$ with respect to the shift σ.

Definition 5. For any sequence of edges $\mathbf{p} \in \widetilde{\mathcal{P}}_n$, its equivalence class with respect to the cyclic shift operator σ is called the *periodic orbit*. The number n is called the *period* of the orbit. Thus the set $\mathcal{P}_n$ is the set of all orbits of period n and $\mathcal{P} = \cup_{n=2}^{\infty} \mathcal{P}_n$. The list of the bonds in the order they are traversed by the orbit $\mathbf{p}$, surrounded by the round brackets, is called the *symbolic code* of the orbit.

Remark 1. The main difference between the periodic orbits and cycles is that a periodic orbit is allowed to pass a bond more than once.

For some periodic orbits $\mathbf{p}$ there is a shorter orbit $\mathbf{q} = (q_1, \dots, q_m)$ of period m, $n = mr$, such that

$$\mathbf{p} = (q_1, \dots, q_m, q_1, \dots, q_m, \dots, q_1, \dots q_m) \tag{2.1.8}$$

Then we say that $\mathbf{p}$ is a *repetition* of the orbit $\mathbf{q}$. The smallest m for which decomposition (2.1.8) is possible is called the *prime period* of $\mathbf{p}$ and the corresponding $r = n/m$ is called the *repetition number*. If $r = 1$ we say that

the orbit is *primitive*. In the above notation each orbit $p \in \mathcal{P}$ corresponds to $m = n/r$ sequences from $\widetilde{\mathcal{P}}$.

Example 4. If we denote $\alpha = (0,1)$, $\beta = (1,2)$, $\gamma = (2,0)$ for the graphs on Fig. 2.1(a), the orbit $(\alpha, \beta, \gamma, \alpha, \beta, \gamma)$ has the period 6, the prime period 3 and the repetition 2. It corresponds to 3 different sequences,

$$[\alpha, \beta, \gamma, \alpha, \beta, \gamma] \tag{2.1.9}$$

$$[\beta, \gamma, \alpha, \beta, \gamma, \alpha] \tag{2.1.10}$$

$$[\gamma, \alpha, \beta, \gamma, \alpha, \beta]. \tag{2.1.11}$$

The graphs we will be considering are metric, that is each bond b has a length, L_b. Naturally, $L_b = L_{\overline{b}}$. Note that we do not consider whether it is geometrically possible to have such a graph, e.g. we do not enforce the triangle inequality.

As a rule, we will be assuming that the different lengths are incommensurate (rationally independent) which means that there are no integers $a_i \neq 0$, such that

$$\sum_i a_i L_{b_i} = 0, \tag{2.1.12}$$

for some bonds $\{b_i\}$. The *length* of an orbit is defined as the sum of lengths of the bonds it passes,

$$l_{\mathbf{p}} = \sum_{i=1}^{n} L_{b_i}, \tag{2.1.13}$$

where $\mathbf{p} = (b_1, \ldots, b_n)$.

If individual lengths are incommensurate then two different orbits have the same length if and only if they pass through the same set of non-directed bonds the same number of times (although in a different order). An obvious consequence of this is that such orbits have the same period.

The simplest example of two orbits of the same length is an orbit and its

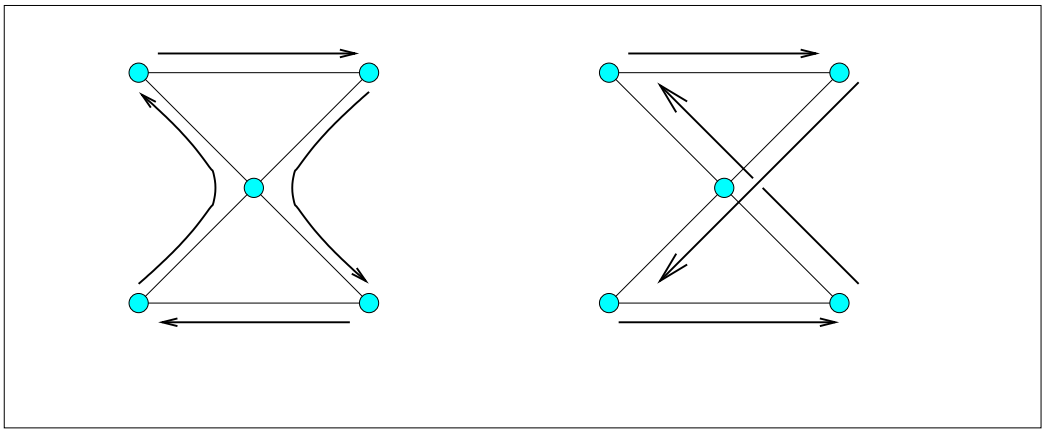

Figure 2.2: Two different orbits with the same length.

reversal:

$$\begin{aligned} \mathbf{p} &= (b_1, b_2, \dots, b_n) \\ \overline{\mathbf{p}} &= \left(\overline{b_n}, \dots, \overline{b_2}, \overline{b_1}\right). \end{aligned} \tag{2.1.14}$$

A less trivial example is shown on Fig. 2.2.

More rigorously, we associate with each orbit a B-dimensional integer vector with nonnegative components

$$\mathbf{p} \mapsto \mathbf{s} \in \mathbb{N}_0^B, \tag{2.1.15}$$

where $\mathbb{N}_0 = \{0, 1, \dots\}$. Here the components s_i indicate the numbers of times the orbit passes through the nondirected bond b_i. Following [25] we call s_i the *bond staying rates*. Then two orbits have the same length if and only if they correspond to the same vector $\mathbf{s}$. Sometimes to indicate that a vector from $\mathbb{N}_0^B$ corresponds to the orbit $\mathbf{p}$ we will write $\mathbf{s}(\mathbf{p})$ instead of just $\mathbf{s}$.

Definition 6. Two orbits belong to the same *degeneracy class* if they have the same length or, equivalently, if they correspond (2.1.15) to the same vector $\mathbf{s}$.

In order to consider functions on the graph we identify each directed bond b with the interval $[0, L_b]$. This gives us a local variable x_b on the bond b; its geometrical meaning is the distance from the initial vertex. Note that if the bond $\bar{b}$ is the reverse of the bond b then $x_{\bar{b}} = L_b - x_b$. The meaning of the

equality sign is that both $x_{\bar{b}}$ and $L_b - x_b$ refer to the same *geometrical* position on the bond. Now one can define a function on a bond and, therefore, define a function on the whole graph as a collection of functions on all bonds of the graph. To ensure that the function is well defined we impose the condition

$$\Psi_b(x_b) = \Psi_{\bar{b}}\,(L_b - x_b) \qquad \text{for all } b \in \mathcal{B}, \tag{2.1.16}$$

where Ψ_b and $\Psi_{\bar{b}}$ are the components of a function Ψ on the whole graph, defined on the directed bonds b and $\bar{b}$ correspondingly. In this way we have that the derivatives depend on the direction of the bond,

$$\Psi_b'(x_b) = -\Psi_{\bar{b}}'\,(L_b - x_b) \qquad \text{for all } b \in \mathcal{B}, \tag{2.1.17}$$

and the integrals do not,

$$\int_0^{L_b} \Psi_b(x_b)dx_b = \int_0^{L_b} \Psi_{\bar{b}}(x_{\bar{b}})dx_b. \tag{2.1.18}$$

One can also define the scalar product of two integrable functions Ψ and Φ as the sum of the integrals

$$\int_0^{L_b} \Psi(x_b)\overline{\Phi(x_b)}dx_b \tag{2.1.19}$$

over all $b \in \mathcal{B}$. This scalar product defines the space $L^2(G)$.

The functions $\Psi \in L^2(G)$ which will be of interest to us are those which are twice differentiable on the bonds (on the endpoints the derivatives are one-sided) with their second derivative being in $L^2(G)$ again. In addition they satisfy the following conditions:

$$\Psi_{(i,j)}(0) = \Psi_{(i,k)}(0) \qquad \text{for any } i, j, k \in \mathcal{V}, \tag{2.1.20}$$

i.e. Ψ is continuous on vertices and

$$\sum_{j:\, C_{i,j}=1} \frac{d}{dx}\Psi_{(i,j)}(0) = 0, \tag{2.1.21}$$

the so-called current conservation condition. The space of all functions satisfying all the above conditions on a graph G we denote by $\mathcal{F}(G)$.

We are interested in the eigenspectrum of the operator $-\frac{d^2}{dx^2}$ acting on the functions from $\mathcal{F}(G)$, namely the numbers $k > 0$ for which the equation

$$-\frac{d^2}{dx^2}\Psi = k^2\Psi, \qquad \Psi \in \mathcal{F}(G) \tag{2.1.22}$$

has a nontrivial solution. We will show that there is a discrete (no accumulation points) unbounded set $\{k_i\}_{i=0}^{\infty} \in \mathbb{R}$ satisfying this condition.

Definition 7. The set of values $\{k_i\}_{i=0}^{\infty}$ for which Eq. (2.1.22) has a solution is called the *quantum spectrum of the graph* G. To underline that we are considering the properties of the quantum spectrum we will sometimes refer to G as *quantum graph*.

It is important to verify that the operator $-\frac{d^2}{dx^2}$ is self-adjoint. Indeed, on a bond b one has

$$\int_0^{L_b} \frac{d^2}{dx_b^2}\Psi_b(x_b)\overline{\Phi_b(x_b)}dx_b = \left[\frac{d\Psi_b}{dx_b}\overline{\Phi_b} - \Psi_b\overline{\frac{d\Phi_b}{dx_b}}\right]_0^{L_b} + \int_0^{L_b}\Psi_b(x_b)\overline{\frac{d^2}{dx_b^2}\Phi_b(x_b)}dx_b. \tag{2.1.23}$$

Substituting the boundary values into the first summand on the right-hand side and remembering Eq. (2.1.17) we obtain

$$\left[\frac{d\Psi_b}{dx_b}\overline{\Phi_b}\right]_0^{L_b} = -\frac{d\Psi_b}{dx_b}(0)\overline{\Phi_b(0)} - \frac{d\Psi_{\bar{b}}}{dx_{\bar{b}}}(0)\overline{\Phi_{\bar{b}}(0)}. \tag{2.1.24}$$

When we sum such expressions over all bonds they cancel due to the conditions (2.1.20) and (2.1.21), for example

$$\begin{aligned}\sum_{b\in\mathcal{B}}\frac{d\Psi_b}{dx_b}(0)\overline{\Phi_b(0)} &= \sum_{(i,j)\in\mathcal{B}}\frac{d\Psi_{(i,j)}}{dx_{(i,j)}}(0)\overline{\Phi_{(i,j)}(0)} \\ &= \sum_{i\in\mathcal{V}}\overline{\Phi_{(i,j)}(0)}\sum_{j\colon(i,j)\in\mathcal{B}}\frac{d\Psi_{(i,j)}}{dx_{(i,j)}}(0) = \sum_{i\in\mathcal{V}}\overline{\Phi_{(i,j)}(0)}\times 0 = 0,\end{aligned} \tag{2.1.25}$$

where we took out the factor $\overline{\Phi_{(i,j)}(0)}$ since it does not depend on j due to condition (2.1.20). Contributions of the second summand of the right-hand side of Eq. (2.1.23) disappear in exactly the same manner. This shows that the operator $-\frac{d^2}{dx^2}$ is symmetric.

It is also clear that in order to have

$$\sum_{b\in\mathcal{B}}\left[\frac{d\Psi_b}{dx_b}\overline{\Phi_b}-\Psi_b\overline{\frac{d\Phi_b}{dx_b}}\right]_0^{L_b}=0 \tag{2.1.26}$$

for a fixed Φ and *any* Ψ satisfying the conditions (2.1.20) and (2.1.21), the functions Φ must satisfy these conditions as well[1] which means that the domain of the definition of the adjoint operator coincides with $\mathcal{F}(G)$. Thus the operator $-\frac{d^2}{dx^2}$ is self-adjoint.

Proposition 1. *The set $\{k_i\}_{i=0}^{\infty}$ is real, unbounded and discrete.*

Proof. The above statement follows from the fact that the operator $-\frac{d^2}{dx^2}$ is self-adjoint and the graph (as the domain of definition of functions from $\mathcal{F}(G)$) is compact (see, for example, [35]). □

2.2 Derivation of the quantization condition

The general solution to Eq. (2.1.22) reads

$$\Psi_{(i,j)}(x)=A_{(i,j)}\exp\{-ikx\}+B_{(i,j)}\exp\{ikx\}\,, \tag{2.2.1}$$

where $A_{(i,j)}$ and $B_{(i,j)}$ are arbitrary coefficients that are to be fixed when we apply the boundary conditions, Eqs. (2.1.20) and (2.1.21).

First of all, imposing condition (2.1.16) we obtain the following relation,

$$B_{(i,j)}=A_{(j,i)}\exp\left\{-ikL_{(i,j)}\right\}. \tag{2.2.2}$$

Then, the current conservation condition at the vertex i, Eq. (2.1.21), gives

$$-ik\left(\sum_j A_{(i,j)}-\sum_j B_{(i,j)}\right)=0. \tag{2.2.3}$$

On the other hand we have the continuity condition, Eq. (2.1.20), which gives

$$A_{(i,j)}+B_{(i,j)}=A_{(i,n)}+B_{(i,n)} \tag{2.2.4}$$

[1] This statement easily follows from the fact that it is possible to construct $\Psi\in\mathcal{F}(G)$ satisfying $\Psi_{(i,j)}(0)=\lambda_i$ and $\frac{d\Psi_b}{dx_b}(0)=\mu_b$ for any given numbers $\{\lambda_i\}$ and $\{\mu_b\}$.

for any vertices j and n adjoint to the vertex i.

For a fixed n we sum equations (2.2.4) over all j adjoint to i:

$$\sum_j A_{(i,j)} + \sum_j B_{(i,j)} = \left(A_{(i,n)} + B_{(i,n)}\right) v_i, \tag{2.2.5}$$

where v_i is the valency of the vertex i. Together with Eq.(2.2.3) it gives

$$2\sum_j A_{(i,j)} = \left(A_{(i,n)} + B_{(i,n)}\right) v_i. \tag{2.2.6}$$

Now we use relation (2.2.2) to eliminate the coefficients $B_{(i,n)}$. Thus we arrive to the equation

$$2\sum_j A_{(i,j)} = v_i \left(A_{(i,n)} + A_{(n,i)} \exp\left\{-ikL_{(i,n)}\right\}\right) \tag{2.2.7}$$

and, therefore,

$$A_{(n,i)} = \exp\left\{ikL_{(n,i)}\right\}\left(\frac{2}{v_i}\sum_j A_{(i,j)} - A_{(i,n)}\right) = D_{(n,i)(n,i)} \sum_{(i,j)} S_{(n,i)(i,j)} A_{(i,j)}. \tag{2.2.8}$$

Here we denoted

$$S_{(n,i)(i,j)} = \frac{2}{v_i} - \delta_{j,n}, \tag{2.2.9}$$

where $\delta_{j,n}$ is the Kronecker delta, and

$$D_{(n,i)(n,i)} = \exp\left\{ikL_{(n,i)}\right\}. \tag{2.2.10}$$

Thus we have a set of linear autonomous equations with respect to the coefficients $A_{(i,j)}$ and we are looking for its nonzero solutions. Equations (2.2.8) can be rewritten as the matrix equation

$$\mathbf{a} = \mathbf{DSa}, \tag{2.2.11}$$

where $\mathbf{a}$ is the vector of the coefficients $A_{(i,j)}$ and $2B \times 2B$ matrices $\mathbf{S}$ and $\mathbf{D}(k)$ are formed out of the matrix elements $D_{(n,i)(n,i)}$ and $S_{(n,i)(i,j)}$ specified by Eqs. (2.2.9) and (2.2.10). The elements of the matrices $\mathbf{S}$ and $\mathbf{D}(k)$ that are not specified are assumed to be zero. Thus we obtain the following matrix condition on k

Theorem 1. *The system of equations (2.1.20)–(2.1.22) has nontrivial solutions if and only if k is a solution of the equation*

$$\det\left(\mathbf{I}-\mathbf{DS}\right)=0, \tag{2.2.12}$$

where the matrix $\mathbf{D}$ *is diagonal with k-dependent elements given by Eq. (2.2.10) and the matrix* $\mathbf{S}$*, with the elements given by Eq. (2.2.9), does not depend on k.*

2.3 Properties of the matrix DS. Trace formula.

The foremost property of the matrix **DS** is unitarity. Indeed, the matrix $\mathbf{D}=e^{ik\mathbf{L}}$, where $\mathbf{L}$ is the diagonal matrix $2B\times 2B$ of lengths L_b, is unitary and the matrix $\mathbf{S}$ is real and can have nonzero elements only in the places corresponding to 1s of the matrix $\mathbf{B}$. Thus the scalar product of (n,i)-th row with (k,l)-th row is always zero if $i\neq l$. Further, the matrix $\mathbf{S}$ has v_i-1 elements $2/v_i$ and one element $2/v_i-1$ in the row (n,i). The number of nonzero elements is independent of n but the position of the element $2/v_i-1$ does depend on n. Therefore if $l=i$ but $k\neq n$ then the corresponding scalar product is equal to

$$\sum_{(l,m)\in\mathcal{B}} S_{(n,i)(l,m)}S_{(k,i)(l,m)}=2\times\frac{2}{v_i}\left(\frac{2}{v_i}-1\right)+(v_i-2)\times\left(\frac{2}{v_i}\right)^2=0. \tag{2.3.1}$$

If both $l=i$ and $k=n$, one gets

$$\sum_{(l,m)\in\mathcal{B}} S^2_{(n,i)(l,m)}=\left(\frac{2}{v_i}-1\right)^2+(v_i-1)\times\left(\frac{2}{v_i}\right)^2=1, \tag{2.3.2}$$

which proves the unitarity of the matrix $\mathbf{S}$.

Since the matrix **DS** is unitary, its eigenvalues have the form $\left\{e^{i\theta_l(k)}\right\}_{l=1}^{2B}$. We would like to prove the estimate

$$0<\min_{b\in\mathcal{B}}L_b\leq\frac{d\theta_l}{dk}\leq\max_{b\in\mathcal{B}}L_b\qquad\text{for all } l=1,\ldots,2B. \tag{2.3.3}$$

Let $|v(k)\rangle$ be the unit eigenvector corresponding to the eigenvalue $e^{i\theta_l(k)}$ (in what follows we omit the subscript l). Differentiating the equation

$$\mathbf{D}(k)\mathbf{S}|v(k)\rangle = e^{i\theta(k)}|v(k)\rangle \tag{2.3.4}$$

with respect to k we obtain

$$\frac{d\mathbf{D}}{dk}\mathbf{S}|v(k)\rangle + \mathbf{DS}|v'(k)\rangle = i\frac{d\theta}{dk}e^{i\theta}|v(k)\rangle + e^{i\theta}|v'(k)\rangle, \tag{2.3.5}$$

where $\frac{d\mathbf{D}}{dk} = i\mathbf{LD}$. Since v is orthogonal to its derivative ($v(k)$ belongs to the unit sphere for all k) and since $\langle v|\mathbf{DS} = e^{-i\theta}\langle v|$, by multiplying Eq. (2.3.5) by $\langle v|$ we arrive to

$$\langle v|i\mathbf{LDS}|v\rangle = \langle v|ie^{i\theta}\frac{d\theta}{dk}v\rangle, \tag{2.3.6}$$

which together with Eq. (2.3.4) leads to

$$\frac{d\theta}{dk} = \langle v|\mathbf{L}|v\rangle = \sum_{b\in\mathcal{B}} L_b|v_b|^2. \tag{2.3.7}$$

The estimate of Eq. (2.3.3) now easily follows.

Theorem 1 tells us that we should be looking for the zeros of the determinant $\det(\mathbf{I}-\mathbf{DS})$. The determinant is zero if and only if one of the eigenvalues of **DS** is equal to 1 or, in other terms, $\theta_l(k) = 0$ modulus 2π for some l. Thus we can write

$$d(k) \equiv \sum_n \delta(k-k_n) = \sum_{l=1}^{2B} \delta_{2\pi}(\theta_l(k))\left|\frac{d\theta_l}{dk}\right|, \tag{2.3.8}$$

where δ is the Dirac delta function and $\delta_{2\pi}$ is the 2π-periodic Dirac delta: $\delta_{2\pi}(x) = \sum_{k=-\infty}^{\infty}\delta(x-2\pi k)$. The function $d(k)$ defined above is called the *spectral density function*. It has the delta peaks at the values of k that we are interested in. Expanding the function $\delta_{2\pi}$ as the Fourier series

$$\delta_{2\pi}(x) = \frac{1}{2\pi}\sum_{n=-\infty}^{\infty} e^{ixn}, \tag{2.3.9}$$

and noticing that the estimate (2.3.3) allows us to remove the modulus sign, we continue

$$\begin{aligned} d(k) &= \frac{1}{2\pi}\sum_{l=1}^{2B}\sum_{n=-\infty}^{\infty} e^{i\theta_l(k)n}\frac{d\theta_l}{dk} \\ &= \frac{1}{2\pi}\frac{d}{dk}\sum_{l=1}^{2B}\theta_l(k) + \frac{1}{2\pi}\frac{d}{dk}\sum_{n=1}^{\infty}\frac{1}{in}\sum_{l=1}^{2B}\left(e^{i\theta_l(k)n} - e^{-i\theta_l(k)n}\right) \\ &= \frac{1}{2\pi}\frac{d}{dk}\sum_{l=1}^{2B}\theta_l(k) + \frac{1}{\pi}\Im\frac{d}{dk}\sum_{n=1}^{\infty}\frac{1}{n}\sum_{l=1}^{2B}e^{i\theta_l(k)n} \\ &= \frac{1}{2\pi}\frac{d}{dk}\sum_{l=1}^{2B}\theta_l(k) + \frac{1}{\pi}\Im\frac{d}{dk}\sum_{n=1}^{\infty}\frac{1}{n}\mathrm{Tr}(\mathbf{DS})^n. \end{aligned} \tag{2.3.10}$$

To simplify the first summand we notice that the determinant of the matrix **DS** is given by

$$\det\mathbf{DS} = e^{ik\sum_{b=1}^{2B}L_b}\det\mathbf{S} = \pm e^{ik\sum_{b=1}^{2B}L_b}. \tag{2.3.11}$$

Alternatively, using the definition of the eigenphases $\{\theta_l\}_{l=1}^{2B}$,

$$\det\mathbf{DS} = e^{i\sum_{l=1}^{2B}\theta_l(k)} \tag{2.3.12}$$

which leads to

$$\frac{d}{dk}\sum_{l=1}^{2B}\theta_l(k) = \sum_{b=1}^{2B}L_b \equiv L. \tag{2.3.13}$$

Now we can expand the traces in the second summand of Eq. (2.3.10) in terms of the matrix elements,

$$\begin{aligned} \mathrm{Tr}(\mathbf{DS})^n &= \sum_{b_1,\ldots,b_n}(\mathbf{DS})_{b_1b_2}(\mathbf{DS})_{b_2b_3}\cdots(\mathbf{DS})_{b_nb_1} \\ &= \sum_{b_1,\ldots,b_n} e^{ik(L_{b_1}+L_{b_2}+\ldots+L_{b_n})}S_{b_1b_2}S_{b_2b_3}\cdots S_{b_nb_1}, \end{aligned} \tag{2.3.14}$$

where $[b_1, b_2, \ldots, b_n]$ are all possible sequences of edges. However since $S_{b_kb_{k+1}}$ is nonzero only if $B_{b_kb_{k+1}} \neq 0$, the only nonzero terms in the sum (2.3.14) correspond to $[b_1, b_2, \ldots, b_n] \in \widetilde{\mathcal{P}_n}$. Introducing the notation

$$A_{\mathbf{p}} \equiv \prod_{i=1}^{n} S_{b_ib_{i+1}}, \qquad \text{where } \mathbf{p} = [b_1, b_2, \ldots, b_n] \text{ and } b_{n+1} = b_1, \tag{2.3.15}$$

we write

$$\mathrm{Tr}(\mathbf{DS})^n = \sum_{\mathbf{p}\in\widetilde{\mathcal{P}_n}} A_{\mathbf{p}} e^{ikl_{\mathbf{p}}} = \sum_{\mathbf{p}\in\mathcal{P}_n} \frac{n}{r_{\mathbf{p}}} A_{\mathbf{p}} e^{ikl_{\mathbf{p}}}, \tag{2.3.16}$$

where the summation now is over the periodic orbits, $l_{\mathbf{p}}$ is the length of the orbit $\mathbf{p}$, Eq. (2.1.13), and $r_{\mathbf{p}}$ is the repetition number of the orbit $\mathbf{p}$.

Substituting this expression for the trace into Eq. (2.3.10) we arrive to what we will refer to as the *trace formula*

$$d(k) \equiv \sum_n \delta(k - k_n) = \frac{L}{2\pi} + \frac{1}{\pi} \sum_{\mathbf{p}\in\mathcal{P}} \frac{l_{\mathbf{p}}}{r_{\mathbf{p}}} A_{\mathbf{p}} \cos(kl_p). \tag{2.3.17}$$

It will provide the basis for our analysis since it establishes a link between the periodic orbits of the graph and its quantum spectrum. To the best of our knowledge, this trace formula was first discovered by Roth [17]. It was then independently derived by Kottos and Smilansky [19, 20] who proceeded to analyse the statistics of the spectrum.

2.4 Geometric meaning of the matrix S

To understand the geometric meaning of the matrix $\mathbf{S}$ it is helpful to represent the general solution to Eq. (2.1.22) in the form

$$\Psi_{(i,j)}(x) = A_{(i,j)} \exp\left\{-ikx_{(i,j)}\right\} + A_{(j,i)} \exp\left\{-ikx_{(j,i)}\right\}, \tag{2.4.1}$$

which is obtained by substitution of Eq. (2.2.2) into Eq. (2.2.1). Thus one can consider the wave on the nondirected bond (i, j) as the superposition of the wave travelling from j to i with the amplitude $A_{(i,j)}$ and the wave travelling from i to j with the amplitude $A_{(j,i)}$.

The wave dynamics is realised through the matrix $\mathbf{DS}$: all the waves $A_{(i,j)}$ arriving to the vertex i contribute to the outgoing amplitude $A_{(n,i)}$ with the weights $S_{(n,i)(i,j)}$. Then, as the wave travels along the bond (i, n), it acquires the phase shift $D_{(n,i)(n,i)}$. The eigenfunctions of the operator $-\frac{d^2}{dx^2}$ are those

functions Ψ (or indeed the vectors of amplitudes $A_{(i,j)}$) which are invariant under the wave dynamics defined above.

If we square the matrix elements of $\mathbf{S}$, i.e. consider the matrix $\mathbf{M}$ with the elements defined by

$$M_{(i,j)(n,i)} = \left|S_{(n,i)(i,j)}\right|^2, \tag{2.4.2}$$

it is easy to see that the matrix $\mathbf{M}$ is stochastic, that is the sum of the elements in each row is equal to 1. Such matrix defines a Markov process on the graph G with $\left|S_{(n,i)(i,j)}\right|^2$ being the probability to go from the bond (i,j) to the bond (n,i). One can consider this process as a classical analogue of our wave dynamics.

It is possible to generalise the matrix $\mathbf{S}$ in the view of the above considerations. Assume without loss of generality that the bonds numbered b_1, b_2, ... , b_{v_i} lead to the vertex i. Let $\mathbf{S}^{(i)}$ be a $v_i \times v_i$ unitary matrix. Then we can put the elements of the matrix $\mathbf{S}^{(i)}$ instead of some elements of $\mathbf{S}$ in the following manner

$$S_{\overline{b_k} b_n} = S^{(i)}_{kn}. \tag{2.4.3}$$

This substitution will not change the unitarity of $\mathbf{S}$ and we can consider the generalised problem [23]

$$\det\left(\mathbf{I} - \mathbf{D}(k)\mathbf{S}\right) = 0, \tag{2.4.4}$$

where $\mathbf{S}$ is now the changed matrix. The matrix $\mathbf{S}^{(i)}$ is then called the *scattering matrix at the vertex i*. The diagonal elements of the matrix $\mathbf{S}^{(i)}$ will be called *reflection (or backscattering) amplitudes* and will be often denoted by r. The off-diagonal will be called *transmission (or normal scattering) amplitudes* and will be denoted by t.

It can be shown that changing the matrix $S^{(i)}$ corresponds to choosing different boundary conditions at the vertex i.

2.5 Smoothed trace formula

The trace formula as shown in Eq. (2.3.17) is exact: the right-hand side is a convergent, in the sense of distributions, series whose sum is equal to the spectral density. However for some mathematical proofs it is more convenient to consider an approximation to the spectral density function which is obtained by smoothing the delta-peaks of the density function.

Let $\eta_\epsilon(k)$ be a family of continuous functions convergent to the Dirac delta function in the sense of distributions as $\epsilon \to 0$. Then the approximate spectral density $d_\epsilon(k)$ is equal to the convolution of the density $d(k)$ with the function $\eta_\epsilon(k)$. As an example we can take

$$\eta_\epsilon(k) = \frac{1}{\sqrt{\pi}\epsilon} e^{-k^2/\epsilon^2} \tag{2.5.1}$$

so that

$$d_\epsilon(k) = \sum_n \frac{1}{\sqrt{\pi}\epsilon} e^{-(k-k_n)^2/\epsilon^2}. \tag{2.5.2}$$

Now the corresponding approximation of the trace formula is also given by the convolution with $\eta_\epsilon(k)$,

$$\begin{aligned} d_\epsilon(k) &= \frac{L}{2\pi} + \frac{1}{\pi} \sum_{\mathbf{p}} \frac{l_{\mathbf{p}}}{r_{\mathbf{p}}} A_{\mathbf{p}} \int_{-\infty}^{\infty} \frac{1}{\sqrt{\pi}\epsilon} \cos\left(l_{\mathbf{p}}\kappa\right) e^{-(k-\kappa)^2/\epsilon^2} d\kappa \\ &= \frac{L}{2\pi} + \frac{1}{\pi} \sum_{\mathbf{p}} \frac{l_{\mathbf{p}}}{r_{\mathbf{p}}} A_{\mathbf{p}} \cos\left(l_{\mathbf{p}}k\right) e^{-l_{\mathbf{p}}^2\epsilon^2/4}. \end{aligned} \tag{2.5.3}$$

Eq. (2.5.3) is easier to handle because the factors $e^{-l_p^2\epsilon^2/4}$ improve the convergence of the series. From the weak convergence (convergence in the sense of distributions) of Eq. (2.3.17) we now move to the uniform convergence for any $\epsilon > 0$.

To see it we write

$$\begin{aligned}
&\left|\sum_{n=N}^{\infty}\sum_{\mathbf{p}\in\mathcal{P}_n}\frac{l_{\mathbf{p}}}{r_{\mathbf{p}}}A_{\mathbf{p}}\cos\left(l_{\mathbf{p}}k\right)e^{-l_{\mathbf{p}}^2\epsilon^2/4}\right| \\
&\qquad\leq\sum_{n=N}^{\infty}\sum_{\ell}\left|\sum_{\substack{\mathbf{p}\in\mathcal{P}_n\\ l_{\mathbf{p}}=\ell}}\frac{l_{\mathbf{p}}}{r_{\mathbf{p}}}A_{\mathbf{p}}\cos\left(l_{\mathbf{p}}k\right)e^{-l_{\mathbf{p}}^2\epsilon^2/4}\right| \\
&\qquad\leq\sum_{n=N}^{\infty}\sum_{\ell}\ell\cos\left(\ell k\right)e^{-\ell^2\epsilon^2/4}\sum_{\substack{\mathbf{p}\in\mathcal{P}_n\\ l_{\mathbf{p}}=\ell}}\left|\frac{A_{\mathbf{p}}}{r_{\mathbf{p}}}\right| \\
&\qquad\leq\sum_{n=N}^{\infty}nL_b^{\max}e^{-(nL_b^{\min})^2\epsilon^2/4}\sum_{\ell}\sum_{\substack{\mathbf{p}\in\mathcal{P}_n\\ l_{\mathbf{p}}=\ell}}\left|\frac{A_{\mathbf{p}}}{r_{\mathbf{p}}}\right| \\
&\qquad\propto\sum_{n=N}^{\infty}nL_b^{\max}e^{-(nL_b^{\min})^2\epsilon^2/4}n^{B-1}, \qquad (2.5.4)
\end{aligned}$$

where we sorted the orbits according to their lengths (i.e. degeneracy classes) and then used the estimates from Appendix A.1 in the last line.

2.6 Spectral statistics

Here we introduce the main objects of our study: the spectral statistics associated with the spectrum of the quantum graphs. The aim of this Section is to express the spectral statistics in the form of sums over periodic orbits with the aid of the trace formula (2.3.17). Although for completeness we include discussions of convergence of the spectral statistics, the material directly relevant to the subsequent investigations is wholly contained in equations (2.6.1), (2.6.5), (2.6.6), (2.6.22), and (2.6.26), (2.6.30). These equations give the definitions and the periodic orbit expansions of the mean density, two-point correlation function and the form factor correspondingly.

2.6.1 Average density

The average (mean) density of the eigenspectrum is defined by

$$\overline{d} \equiv \langle d(k) \rangle_k \equiv \lim_{T\to\infty} \frac{1}{T} \int_0^T d(k) dk \tag{2.6.1}$$

and its meaning is the average number of the eigenvalues k_n per interval of unit length.

Define

$$\overline{d}(T) = \frac{1}{T} \int_0^T d(k) dk \tag{2.6.2}$$

$$\overline{d_\epsilon}(T) = \frac{1}{T} \int_0^T d_\epsilon(k) dk. \tag{2.6.3}$$

We include the following Proposition without proof.

Proposition 2. *If the function η_ϵ is such that $\int \eta_\epsilon(x)dx = 1$ and $\eta_\epsilon(x) > 0$ for all x then for the corresponding d_ϵ,*

$$\lim_{T\to\infty} \overline{d_\epsilon}(T) = \lim_{T\to\infty} \overline{d}(T). \tag{2.6.4}$$

The equality of the limits here means that the limits either both do not exist or both exist and are equal.

Now we can integrate the series (2.5.3) and take the limit termwise (we can do it since the series is uniformly convergent) to obtain

$$\overline{d} = \frac{L}{2\pi}, \tag{2.6.5}$$

where $L = \sum_{b\in\mathcal{B}} L_b$. In the following we will usually rescale the spectral density, i.e. consider $\frac{1}{\overline{d}} d\left(\frac{k}{\overline{d}}\right)$. The mean spacing between two eigenvalues of such rescaled density is equal to one.

2.6.2 Two-point correlation function

The two-point correlation function is defined by

$$\begin{aligned} R_2(x) &\equiv \left(\frac{2\pi}{L}\right)^2 \left\langle d(k) d\left(k + \frac{2\pi x}{L}\right) \right\rangle_k \\ &\equiv \left(\frac{2\pi}{L}\right)^2 \lim_{T\to\infty} \frac{1}{T} \int_0^T d(k) d\left(k + \frac{2\pi x}{L}\right) dk. \end{aligned} \tag{2.6.6}$$

As it can easily be shown from the definition, the function R_2 is even.

If we assume, for simplicity, that $L = 2\pi$ then the two-point correlation function $R_2(x)$ can be also expressed as

$$R_2(x) = \lim_{M\to\infty} \frac{1}{M} \sum_{m=0}^{M} \sum_{n=0}^{\infty} \delta\Big(x - (k_n - k_m)\Big), \tag{2.6.7}$$

or it can be defined by its action on a test function $h(x)$,

$$\langle h, R_2\rangle = \lim_{M\to\infty} \frac{1}{M} \sum_{m=0}^{M} \sum_{n=0}^{\infty} h(k_n - k_m). \tag{2.6.8}$$

From these equalities the meaning of the function $R_2(x)$ can be easily understood. For example, if we take $h(x)$ to be normalised characteristic function of an interval[2], one can see that $\langle h, R_2\rangle$ counts the average number of couples of eigenvalues whose difference lies in the interval. Basing on Eq. (2.6.7) one can also say that $R_2(x)$ is the density function of all possible differences of eigenvalues.

We define the smoothed two-point correlation function by

$$R_{2,\epsilon}(x) \equiv \left(\frac{2\pi}{L}\right)^2 \lim_{T\to\infty} \frac{1}{T} \int_0^T d_\epsilon(k) d_\epsilon\left(k + \frac{2\pi x}{L}\right) dk \tag{2.6.9}$$

where $d_\epsilon(k) = \sum_n \eta_\epsilon(k - k_n)$ with $\eta_\epsilon(k) \to \delta(k)$ as $\epsilon \to 0$.

A proposition similar to Proposition 2 can be formulated for the two-point correlation function.

Proposition 3. *Let $\delta(k) = \lim_{\epsilon\to 0} \eta_\epsilon(k)$, with $\eta_\epsilon(k)$ continuous and nonnegative. If there exists the average density $\overline{d}$ and if the function $R_{2,\epsilon}(x)$, as defined by Eq. (2.6.9), exists for some ϵ_0 then it exists for all ϵ and*

$$\lim_{\epsilon\to 0} (R_{2,\epsilon}(x) - R_2(x)) = 0 \tag{2.6.10}$$

in the weak sense.

[2]although it is not a test function, under certain conditions Eq. (2.6.8) will still make sense

Proof. We will give a schematic proof for the case when the approximating functions η_ϵ have compact support. If we additionally require that η_ϵ are from C^∞ than their convolution with $\cos(l_{\mathbf{p}}k)$ will produce factors decaying expronentially fast with $l_{\mathbf{p}}$. Such factors will play the role of $e^{-l_{\mathbf{p}}^2\epsilon^2/4}$ in a proof like in Eq. (2.5.4).

Let the functions η_ϵ have their support inside the interval $[-a,a]$. We also assume, for simplicity, that $L = 2\pi$.

Then for a fixed x and ϵ we can estimate

$$\begin{aligned} \frac{1}{T} \sum_{\substack{a<k_m<T-a \\ a<x+k_n<T-a}} \chi_\epsilon(x-(k_n-k_m)) &\leq \frac{1}{T}\int_0^T d_\epsilon(k)d_\epsilon(k+x)dk \qquad (2.6.11) \\ &\leq \frac{1}{T} \sum_{\substack{-a<k_m<T+a \\ -a<x+k_n<T+a}} \chi_\epsilon(x-(k_n-k_m)), \end{aligned}$$

where

$$\chi_\epsilon(k) = \int_{-\infty}^{\infty} \eta_\epsilon(\lambda)\eta_\epsilon(\lambda+k)d\lambda. \qquad (2.6.12)$$

The function χ_ϵ is bounded thus the difference between the left and the right estimate in Eq. (2.6.11) is in the number of the eigenvalues in two intervals, $[-a,a]$ and $[T-a,T+a]$. Such number, divided by T, must decrease to zero as $T\to\infty$ (otherwise the average density $\overline{d}$ would not exist). Thus we have

$$R_{2,\epsilon}(x) = \lim_{M\to\infty} \frac{1}{M} \sum_{m=0}^{M}\sum_{n=0}^{\infty} \chi_\epsilon\left(x-(k_n-k_m)\right), \qquad (2.6.13)$$

The functions $\chi_\epsilon(k)$ have support in the interval $[-2a,2a]$ and also converge to delta functions as $\epsilon\to 0$.

Introduce the notation

$$F_\epsilon(M,x) = \sum_{m=0}^{M}\sum_{n=0}^{\infty} \chi_\epsilon\left(x-(k_n-k_m)\right), \qquad (2.6.14)$$

$$F(M,x) = \sum_{m=0}^{M}\sum_{n=0}^{\infty} \delta\left(x-(k_n-k_m)\right). \qquad (2.6.15)$$

We would like to prove that for any test function $h(x)$ with support in $[-b,b]$,

$$\lim_{\epsilon\to 0}\left[\lim_{M\to\infty}\frac{1}{M}\Big\langle F(M,x)-F_\epsilon(M,x),\ h(x)\Big\rangle\right] = 0. \qquad (2.6.16)$$

Since the functions $\chi_\epsilon(k)$ approximate $\delta(k)$, we have

$$|\langle \delta(x-k) - \chi_\epsilon(x-k), h(x)\rangle| \le \alpha(\epsilon) \to 0, \tag{2.6.17}$$

as $\epsilon \to 0$ for any fixed $h(x)$ and for all values of the shift k.

Now we can estimate

$$\left| \left\langle F(M,x) - F_\epsilon(M,x),\ h(x) \right\rangle \right| < N(M)\alpha(\epsilon), \tag{2.6.18}$$

where $N(M)$ is the number of pairs k_n, k_m such that the support of the function $\chi_\epsilon\left(x-(k_n-k_m)\right)$ overlaps with support of $h(x)$. In other words, it is number of pairs of eigenvalues k_n, k_m such that $m < M$ and $k_n - k_m \in [-2a-b, 2a+b]$. The existence of $R_{\epsilon_0}(x)$ for some ϵ_0 implies that $\lim_{M\to\infty} N(M)/M$ is bounded. This remark proves Eq. (2.6.16). □

Using Proposition 3, we substitute Eq. (2.5.3) into definition (2.6.9) to obtain

$$\begin{aligned} R_{2,\epsilon}(x) \;=\; & \left(\frac{2\pi}{L}\right)^2 \lim_{T\to\infty} \frac{1}{T} \int_0^T \left[\frac{L}{2\pi} \left(d_\epsilon(k) + d_\epsilon\left(k + \frac{2\pi x}{L}\right) - \frac{L}{2\pi} \right) \right. \\ & \left. + \frac{1}{\pi^2} \sum_{\mathbf{p},\mathbf{q}} \frac{l_\mathbf{p} l_\mathbf{q}}{r_\mathbf{p} r_\mathbf{q}} A_\mathbf{p} A_\mathbf{q} \cos\left(l_\mathbf{p} k\right) \cos\left(l_\mathbf{q} k + l_\mathbf{q} \frac{L}{2\pi} \right) e^{-\left(l_\mathbf{p}^2 + l_\mathbf{q}^2\right)\epsilon^2/4} \right] dk, \end{aligned} \tag{2.6.19}$$

where the double series in the second line is uniformly convergent with respect to k. The integration of the summand in the first line produces (c.f. Subsection 2.6.1)

$$\frac{2\pi}{L}\left(\overline{d} + \overline{d} - \frac{L}{2\pi}\right) = 1, \tag{2.6.20}$$

while in the second line we expand the product of cosines

$$\begin{aligned} \cos\left(l_\mathbf{p} k\right) \cos\left(l_\mathbf{q} k + l_\mathbf{q} \frac{2\pi x}{L} \right) = \frac{1}{2} \left[\cos\left((l_\mathbf{q} - l_\mathbf{p}) k + l_\mathbf{q} \frac{2\pi x}{L} \right) \right. \\ \left. + \cos\left((l_\mathbf{p} + l_\mathbf{q}) k + l_\mathbf{q} \frac{2\pi x}{L} \right) \right]. \end{aligned} \tag{2.6.21}$$

Now when we integrate and take the termwise limit, the only terms left will be those which had the coefficient of k in the cosine being equal to zero. Thus

from the double sum only the pairs of periodic orbits with equal length will survive,

$$\begin{aligned} R_{2,\epsilon}(x) &= 1 + \frac{2}{L^2} \sum_{\mathbf{p},\mathbf{q}\in\mathcal{P}} \frac{l_\mathbf{p} l_\mathbf{q}}{r_\mathbf{p} r_\mathbf{q}} A_\mathbf{p} A_\mathbf{q} \cos\left(l_\mathbf{q} \frac{2\pi x}{L}\right) e^{-\left(l_\mathbf{p}^2 + l_\mathbf{q}^2\right)\epsilon^2/4} \delta_{l_\mathbf{p}, l_\mathbf{q}} \\ &= 1 + \frac{2}{L^2} \sum_{\mathbf{s}} \ell^2 \cos\left(l_\mathbf{q} \frac{2\pi x}{L}\right) e^{-\ell^2\epsilon^2/2} \left(\sum_{\mathbf{s}(\mathbf{p})=\mathbf{s}} \frac{A_\mathbf{p}}{r_\mathbf{p}}\right)^2, \quad (2.6.22) \end{aligned}$$

where ℓ is the length of the periodic orbits from the degeneracy class $\mathbf{s}$ and the symbol $\delta_{l_\mathbf{p}, l_\mathbf{q}}$ is equal to 1 if $l_\mathbf{p} = l_\mathbf{q}$ and is 0 otherwise. Using Theorems 3 and 4 from Appendix A.1 one can show that the series in Eq. (2.6.22) is convergent uniformly in x for any value of $\epsilon > 0$. Thus $R_{2,\epsilon}(x)$ exists and converges to $R_2(x)$ as $\epsilon \to 0$.

Remark 2. The main (and only) effect of the averaging

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T \cdot \, dk, \quad (2.6.23)$$

was to remove the cosines, as in Eq. (2.6.21), when $l_\mathbf{p} \neq l_\mathbf{q}$ and thus restrict the summation in (2.6.22) to the pairs of orbits of the same length. Another way to achieve this is to average with respect to individual bond lengths and then send k to infinity,

$$\lim_{k\to\infty} \int_{L_0}^{L_0+\Delta L} \cdots \int_{L_0}^{L_0+\Delta L} \cos\left((l_\mathbf{q} - l_\mathbf{p})k + \alpha\right) \frac{dL_1}{\Delta L} \cdots \frac{dL_B}{\Delta L} = \delta_{l_\mathbf{p}, l_\mathbf{q}} \cos\alpha. \quad (2.6.24)$$

The above follows from the representations

$$l_\mathbf{p} = \sum_{i=0}^{B} s_i(\mathbf{p}) L_i, \qquad l_\mathbf{q} = \sum_{i=0}^{B} s_i(\mathbf{q}) L_i, \quad (2.6.25)$$

where $s_i(\mathbf{p})$ is the staying rate of the orbit $\mathbf{p}$ on the ith bond, and the fact that unless $s_i(\mathbf{p}) = s_i(\mathbf{q})$, the integration with respect to L_i will produce a factor of order k^{-1}. Thus the averaging defined in (2.6.24) is formally equivalent to averaging (2.6.23), although it is hard to justify it more rigorously. Averaging (2.6.24) will be employed in Chapter 5.

2.6.3 The form factor

Another function associated with the spectrum is the form factor $K(\tau)$. The form factor $K(\tau)$ is the Fourier transform (in the generalised sense) of the two-point correlation function

$$K(\tau) \equiv \int_{-\infty}^{\infty} (R_2(x) - 1) \exp(2\pi i x \tau) dx. \tag{2.6.26}$$

Since the Fourier transform is continuous, we can write $K(\tau) = \lim_{\epsilon \to 0} K_\epsilon(\tau)$, where

$$K_\epsilon(\tau) \equiv \int_{-\infty}^{\infty} (R_{2,\epsilon}(x) - 1) \exp(2\pi i x \tau) dx. \tag{2.6.27}$$

Taking the Fourier transform termwise using

$$\int_{-\infty}^{\infty} e^{2\pi i x \tau} \cos\left(\frac{2\pi x l_{\mathbf{p}}}{L}\right) dx = \frac{1}{2}\delta\left(\tau + \frac{l_{\mathbf{p}}}{L}\right) + \frac{1}{2}\delta\left(\tau - \frac{l_{\mathbf{p}}}{L}\right), \tag{2.6.28}$$

we arrive to

$$K_\epsilon(\tau) = \frac{1}{L^2} \sum_{\mathbf{p},\mathbf{q} \in \mathcal{P}} \frac{l_{\mathbf{p}}}{r_{\mathbf{p}}} \frac{l_{\mathbf{q}}}{r_{\mathbf{q}}} A_{\mathbf{p}} A_{\mathbf{q}} \delta\left(\tau - \frac{l_{\mathbf{p}}}{L}\right) e^{-\left(l_{\mathbf{p}}^2\right)\epsilon^2/2} \delta_{l_{\mathbf{p}}, l_{\mathbf{q}}}, \tag{2.6.29}$$

for $\tau > 0$ (the form factor is even: $K(-\tau) = K(\tau)$). Now we can take the limit $\epsilon \to 0$ termwise to finally obtain the periodic orbit expansion of the form factor,

$$K(\tau) = \frac{1}{L^2} \sum_{\mathbf{p},\mathbf{q} \in \mathcal{P}} \frac{l_{\mathbf{p}}}{r_{\mathbf{p}}} \frac{l_{\mathbf{q}}}{r_{\mathbf{q}}} A_{\mathbf{p}} A_{\mathbf{q}} \delta\left(\tau - \frac{l_{\mathbf{p}}}{L}\right) \delta_{l_{\mathbf{p}}, l_{\mathbf{q}}}. \tag{2.6.30}$$

In the next chapter we derive an expansion for the form-factor for star-graphs (see Example 3) starting with Eq. (2.6.30) and then "enumerating" the periodic orbits and the degeneracy classes.

Chapter 3

Form-factor for the star graphs

In this chapter we study the form-factor $K(\tau)$ (defined by Eqs. (2.6.26-2.6.30)) in the limit $B \to \infty$ for a special family of graphs, known as *star graphs*. These are graphs with $B+1$ vertices marked 0 to B and with the set of bonds $\mathcal{B} = \{(0,i),(i,0) : i = 1 \dots B\}$; see Fig. 2.1. For simplicity we shall number the (nondirected) bonds by the number of their outward endvertex. For star graphs the valency of the vertex 0 is B and the valency of the other vertices is 1 which significantly simplifies the matrix $\mathbf{S}$; for example, the backscattering from the vertices $1 \dots v$ has the weight 1. We shall call such backscatterings *trivial*. As for the transitions through the vertex 0, the backscattering has the weight $r = \frac{B-2}{B}$ while normal scattering has the weight $t = 2/B$. Thus it is clear that in the limit $B \to \infty$ the leading-order contributions come from orbits with the maximum number of nontrivial backscatterings. This will form the basis of our analysis.

3.1 Expansion of the form factor

3.1.1 General formulae

In Section 2.6.3 we derived an expansion of the form-factor in terms of the periodic orbits,

$$K(\tau) = \frac{1}{L^2} \sum_{n=2}^{\infty} \sum_{\mathbf{p},\mathbf{q} \in \mathcal{P}_n} \frac{l_\mathbf{p}}{r_\mathbf{p}} \frac{l_\mathbf{q}}{r_\mathbf{q}} A_\mathbf{p} A_\mathbf{q} \delta \left(\tau - \frac{l_\mathbf{p}}{L} \right) \delta_{l_\mathbf{p}, l_\mathbf{q}}, \tag{3.1.1}$$

when $\tau > 0$ (K is an even function). Loosely speaking, the form factor is a sum of delta-functions positioned at the lengths of the periodic orbits and weighted by the factors $A_\mathbf{p}$. A very important factor in Eq. (3.1.1) is the coupling between different orbits of the same length which is present due to the Kronecker delta. It shows that the contribution comes only from the couples of orbits $\mathbf{p}$ and $\mathbf{q}$ which belong to the same degeneracy class.

Let us consider the contribution of a particular degeneracy class characterised by the length ℓ of its orbits,

$$\sum_{\mathbf{p},\mathbf{q}:\, l_\mathbf{p} = l_\mathbf{q} = \ell} \frac{\ell}{r_\mathbf{p}} \frac{\ell}{r_\mathbf{q}} A_\mathbf{p} A_\mathbf{q} \delta \left(\tau - \frac{\ell}{L} \right) = \ell^2 \delta \left(\tau - \frac{\ell}{L} \right) \left(\sum_{\mathbf{p} \in \mathcal{P}_n :\ \ l_\mathbf{p} = \ell} \frac{A_\mathbf{p}}{r_\mathbf{p}} \right)^2 . \tag{3.1.2}$$

This allows us to write

$$K(\tau) = \frac{1}{L^2} \sum_{n=2}^{\infty} \sum_{\ell} \ell^2 \delta \left(\tau - \frac{\ell}{L} \right) \left(\sum_{\mathbf{p} \in \mathcal{P}_n,\ l_\mathbf{p} = \ell} \frac{A_\mathbf{p}}{r_\mathbf{p}} \right)^2 , \tag{3.1.3}$$

where the first (outmost) sum is over all periods, the second is over all degeneracy classes, parametrised here by the length ℓ, and the last is over the orbits within the degeneracy class.

In this Chapter we aim to calculate the weak limit of $K(\tau)$ as $B \to \infty$ and our approach is best described with the aid of Fig. (3.1). On the schematic drawing of the form factor for a $B = 3$ star graph the individual lengths of the bonds are chosen in such a way that the delta functions corresponding to the degeneracy classes of the period $2k$ (on star graphs all orbits have even period)

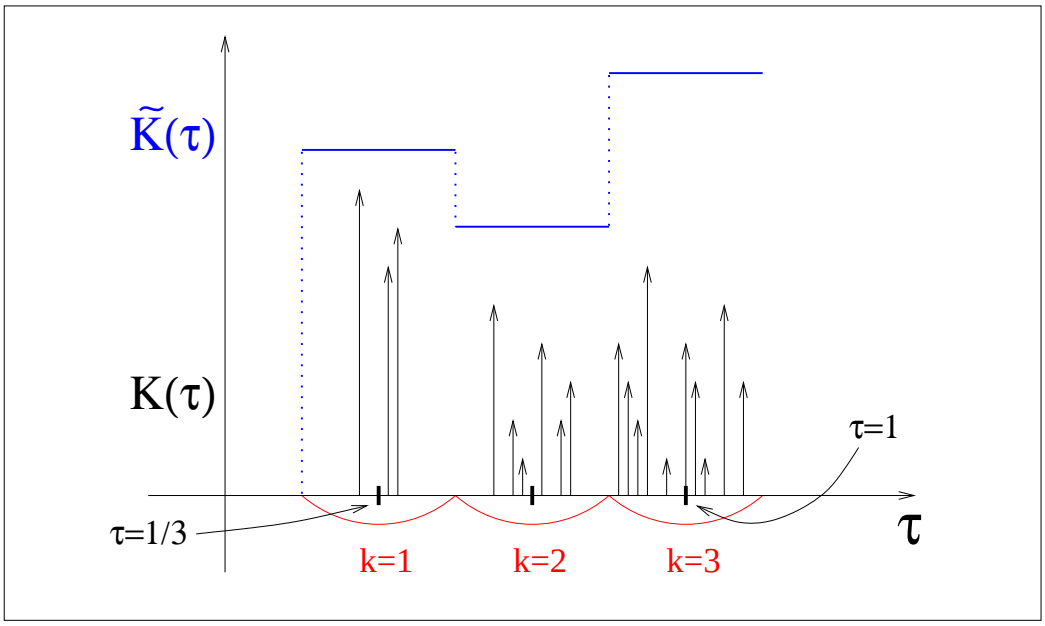

Figure 3.1: Schematic plot of the form factor $K(\tau)$ and its approximation $\widetilde{K}(\tau)$ for a 3-star graph. The delta functions are denoted by arrows pointing up.

are clustered around the point k/B. Then we can integrate $K(\tau)$ against the characteristic functions of the intervals of the size $1/B$ around these points obtaining the staircase approximation to the form factor which we denote by $\widetilde{K}(\tau)$. Each step in $\widetilde{K}(\tau)$ collects in itself all contributions from orbits of the same period. It is easy to see that $\widetilde{K}(\tau)$ and $K(\tau)$ have the same weak limit as $B \to \infty$, therefore it is enough to study the approximation $\widetilde{K}(\tau)$. The condition on the bonds lengths and the details of the integration are described below.

We assume that the individual lengths of the edges are densely distributed around their average, which, without loss of generality, we take to be unity. Picking the lengths at random does not contradict our usual condition that the lengths should be incommensurate. In fact, having commensurate lengths is an event of zero probability.

For example, we can use the uniform distribution on the interval $[1 - 1/(2B), 1 + 1/(2B)]$ in such a way that $L = 2B$. Note that the distribution changes with the valency B. This is done in such a way that the orbits of period

$2k$ have their lengths distributed in the interval $[2k - k/B, 2k + k/B]$ and, therefore, when $k/B \leq 1$ the corresponding delta functions are concentrated in the interval

$$\left[\frac{k}{B} - \frac{k}{2B^2}, \frac{k}{B} + \frac{k}{2B^2}\right] \subset \left[\frac{k}{B} - \frac{1}{2B}, \frac{k}{B} + \frac{1}{2B}\right]. \tag{3.1.4}$$

Thus the contribution from orbits of different period will be confined to non-intersecting intervals if $k < B$. To approximate the form factor around k/B we integrate it against the characteristic function of the corresponding interval $\left[\frac{k}{B} - \frac{1}{2B}, \frac{k}{B} + \frac{1}{2B}\right]$ and divide by the length $1/B$ of the interval. This contribution is equal to

$$\widetilde{K}(\tau) = \frac{B}{L^2} \sum_{\ell} \ell^2 \left(\sum_{\mathbf{p} \in \mathcal{P}_{2k},\ l_{\mathbf{p}} = \ell} \frac{A_{\mathbf{p}}}{r_{\mathbf{p}}} \right)^2 \tag{3.1.5}$$

for $\tau \in \left[\frac{k}{B} - \frac{1}{2B}, \frac{k}{B} + \frac{1}{2B}\right]$. As mentioned above, $\widetilde{K}(\tau)$ and $K(\tau)$ have the same weak limit $K^{lim}(\tau)$ as $B \to \infty$ in the sense of distributions. In what will follow, to determine the value of the form factor K at a point τ we will send both B and k to infinity in such a way that $\lim k/B = \tau$.

Under the above conditions on the distribution of the lengths, the form factor $K(k/B)$ is well approximated by another quantity, $\langle |\mathrm{Tr}\mathbf{S}^{2k}|^2 \rangle/(2L)$, the periodic orbit expansion for which can be obtained from (3.1.5) by substituting $\ell = 2k$. In what follows we make the approximation $\ell \approx 2k$ (*i.e.* consider $\langle |\mathrm{Tr}\mathbf{S}^{2k}|^2 \rangle/(2L)$ instead of $K(k/B)$) but still refer to the resulting expression as the form factor.

Since the star graphs are special we will have to change the conventions we introduced in Chapter 2, in order to simplify notation. For each orbit the number of traversals of a given bond is even so throughout this Chapter we will count the traversals in one direction only, e.g. from the centre to periphery. As before, each degeneracy class will be marked by a vector $\mathbf{s}$. However now the component s_i of the vector $\mathbf{s}$ is the number of traversals of the bond i in the *outward direction*. When we write a symbolic code for an orbit $\mathbf{p}$, we also

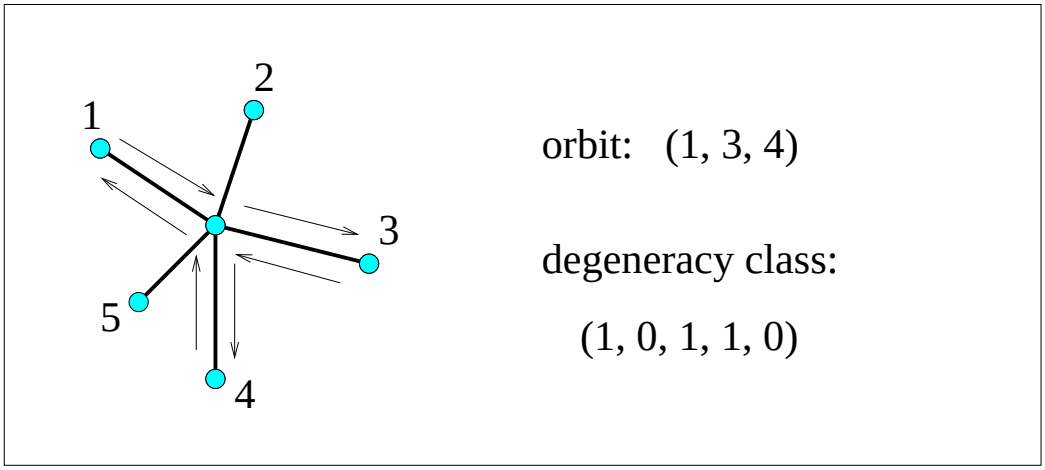

Figure 3.2: An example of simplified notation for the periodic orbit and the corresponding degeneracy class.

list only traversals of a bond in the outward direction. For example to denote the orbit passing through the bonds $(0,1)$, $(1,0)$, $(0,3)$, $(3,0)$, $(0,4)$ and $(4,0)$ successively, as depicted in Fig. 3.2, we will use the simplified notation $(1,3,4)$. Clearly this information is sufficient to identify the orbit.

We start by dividing all orbits into B groups, based on the number j of *different* edges the orbit traverses. This number is an invariant of the degeneracy class; thus the sums over the degeneracy classes will remain intact. We will be interested in the degeneracy classes with exactly j nonzero components in their vector $\mathbf{s}$ and with $|\mathbf{s}| = \sum_{i=1}^{v} s_i = k$, the half-period. Thus, writing the symbolic code for an orbit $\mathbf{p}$ from such a degeneracy class, we get a sequence of k symbols of j different types. When we calculate the weight $A_{\mathbf{p}}$ of the orbit, Eq. (2.3.15), each pair of different symbols standing next to each other contributes the factor $t = 2/B$ to $A_{\mathbf{p}}$ and each pair of identical symbols gives $r = 2/B - 1$. These contributions multiply together to produce $A_{\mathbf{p}}$, for example the orbit $(1,1,2,2,1,3)$ gives

$$A_{\mathbf{p}} = t^4 r^2 = \left(\frac{2}{B}\right)^4 \left(\frac{2}{B} - 1\right)^2 . \tag{3.1.6}$$

Note that the transition between last 3 and first 1 is also contributing. A very important feature of an orbit is the number of *groups* of identical symbols standing next to each other. For example, the orbit $(1,1,2,2,1,3)$ has two

groups of "1"s, one group of "2"s and one of "3"s. On the other hand, due to the cyclicity, the orbit $(1,2,2,1)$ has only one group of "1"s. It is clear that the number of transitions of the orbit *through* the central vertex (thus contributing the factor t) is given by the total number of the groups[1]. Thus to calculate the contribution from a degeneracy class, it is necessary to know the number of orbits in this degeneracy class that have g_i groups of the symbol "i" in their representation, $i = 1, \ldots, j$. We denote such number by $N^{g_1,\ldots,g_j}_{s_1,\ldots,s_j}$. Then we can write for the contribution of a degeneracy class $\mathbf{s}_0$

$$\sum_{\mathbf{s}(\mathbf{p})=\mathbf{s}_0} \frac{A_\mathbf{p}}{r_\mathbf{p}} = \sum_{g_1=1}^{s_1} \cdots \sum_{g_j=1}^{s_j} N^{g_1,\ldots,g_j}_{s_1,\ldots,s_j} t^G r^{k-G}, \tag{3.1.7}$$

where $G = \sum_{i=1}^{j} g_i$ is the total number of groups. In order for Eq. (3.1.7) to be exact, the number $N^{g_1,\ldots,g_j}_{s_1,\ldots,s_j}$ should take into account the repetitions, i.e. count an orbit which is a repetition of another orbit not as 1 but as $1/r_\mathbf{p}$.

We now rewrite the contribution of the degeneracy class $\mathbf{s}$ in the form

$$\sum_{s(\mathbf{p})=\mathbf{s}} \frac{A_\mathbf{p}}{r_\mathbf{p}} = r^k (t/r)^j \sum_{g_1=1}^{s_1} \cdots \sum_{g_j=1}^{s_j} N^{g_1,\ldots,g_j}_{s_1,\ldots,s_j} (t/r)^{G-j} = r^k (t/r)^j D_\mathbf{s}(B) \tag{3.1.8}$$

and thus obtain from Eq. (3.1.5)

$$\begin{aligned} K^{lim}(\tau) = \lim_{B\to\infty} \widetilde{K}(\tau) &= \lim_{B\to\infty} \frac{B}{L^2} \sum_\mathbf{s} (2k)^2 r^{2k} (t/r)^{2j} D^2_\mathbf{s}(B) \\ &= K_1(\tau) + \lim_{B\to\infty} \frac{B}{L^2} \sum_{j=2}^{\infty} (2k)^2 \binom{B}{j} \left(\frac{B-2}{B}\right)^{2k} \left(\frac{2}{B-2}\right)^{2j} H_j(B) \\ &\equiv \sum_{j=1}^{\infty} K_j(\tau), \end{aligned} \tag{3.1.9}$$

where

- the term for $j = 1$ is slightly different and has to be treated separately,
- $L = 2B$ is the total length of the graph,
- $(2k)^2$ is the approximate squared length of the orbits,

[1] The only exception to this rule are the orbits which have 1 group in total, that is the orbits that are confined to one edge. Such orbits do not have factors t in their coefficient $A_\mathbf{p}$

- the binomial coefficient $\binom{B}{j}$ is the number of ways to choose j traversed edges out of the available B,

- and

$$H_j(B) = \sum_{|\mathbf{s}|=k} D_{\mathbf{s}}^2(B) \tag{3.1.10}$$

is the sum over all degeneracy classes $\mathbf{s} \in \mathbb{N}^j$ with all j components nonzero.

Taking the limit as $B \to \infty$ in Eq. (3.1.9) termwise and with $\tau = k/B$ fixed, we find

$$K^{lim}(\tau) = \lim_{B\to\infty} \widetilde{K}(\tau) = K_1(\tau) + \sum_{j=2}^{\infty} \frac{4^j}{j!} H_j \tau^2 \exp(-4\tau), \tag{3.1.11}$$

where $H_j = \lim_{B\to\infty} B^{1-j} H_j(B)$ and the limit

$$\lim_{B\to\infty} \left(\frac{B-2}{B}\right)^{2k} = \lim_{B\to\infty} \left(1 - \frac{1}{B/2}\right)^{4\tau B/2} = \exp(-4\tau) \tag{3.1.12}$$

was used.

3.1.2 Calculation of $K_1(\tau)$

$K_1(\tau)$ is the contribution from the orbits which are confined to only one edge. All factors in $K_1(\tau)$ are the same as for general j, with the exception that the factor $\left(\frac{2}{B-2}\right)^{2j}$ disappears altogether. Indeed, the weight of an orbit which passes through only one bond is r^k, not $r^{k-1}t$. The number of orbits in a degeneracy class is obvious for $j = 1$, it is $N_{s_1}^{g_1} = 1/k$ for $g_1 = 1$ and 0 otherwise (here $s_1 = k$). This number takes into account the repetitions: there is only one orbit and it has $r_{\mathbf{p}} = k$.

Adjusting the formula in Eq. (3.1.9) we obtain

$$K_1(\tau) = \lim_{B\to\infty} \left[\frac{B}{L^2}(2k)^2 B \left(\frac{B-2}{B}\right)^{2k} \left(\frac{1}{k}\right)^2\right] = \exp\left(-4\tau\right), \tag{3.1.13}$$

where $\tau = k/B$ was held fixed.

As we shall see later this is the dominant contribution for small τ: the next contribution coming form the orbits which traverse only 2 different bonds is of order τ^3 as $\tau \to 0$.

3.1.3 The $j = 2$ contribution

The $j = 2$ contribution is relatively simple and can be considered separately to illustrate our approach. It has the form

$$K_2(\tau) = \frac{4^2}{2!}\tau^2 \exp(-4\tau) H_2 \tag{3.1.14}$$

where $H_2 = \lim_{B\to\infty} \frac{H_2(B)}{B}$ is the quantity we now want to calculate. Writing out the formula for $H_2(B)$ we arrive to

$$H_2 = \lim_{B\to\infty} \frac{1}{B} \sum_{s_1=1}^{k-1} D^2_{(s_1,k-s_1)}, \tag{3.1.15}$$

with $D_{(s_1,s_2)}(B)$ being the contribution from orbits which traverses only two edges s_1 and s_2 times respectively. Now we make use of the fact that as $B \to \infty$ the sum can be replaced by an integral, so that

$$H_2 = \int_0^\tau D^2(q_1, \tau - q_1) dq_1, \tag{3.1.16}$$

where $D(q_1, q_2)$ is the $B \to \infty$ limit of $D_{(s_1,s_2)}(B)$, $q_i = s_i/B$ and $\tau = k/B$, as before. $D_{(s_1,s_2)}(B)$ can be expanded as

$$\begin{aligned} &D_{(s_1,s_2)}(B) \\ &\quad = 1 + \frac{1}{2} b(s_1,2) b(s_2,2) \left(\frac{2}{B-2}\right)^2 + \frac{1}{3} b(s_1,3) b(s_2,3) \left(\frac{2}{B-2}\right)^4 + \dots \\ &\qquad\qquad = \sum_{g=1}^{\infty} \frac{1}{g} b(s_1,g) b(s_2,g) \left(\frac{2}{B-2}\right)^{2g-2}, \end{aligned} \tag{3.1.17}$$

where $2/(B-2) = -t/r$ and $b(s,g) = \binom{s-1}{g-1}$ is the number of partitions of an interval of length s into g non-intersecting subintervals of integer length (see Section A.2 for the derivation). The idea of the decomposition is based on the

fact that a $j = 2$ orbit may be represented in general as

$$(\underbrace{1,\ldots,1}_{a_1},\overbrace{2,\ldots,2}^{b_1},\underbrace{1,\ldots,1}_{a_2},\ldots,\underbrace{1,\ldots,1}_{a_g},\overbrace{2,\ldots,2}^{b_g}), \tag{3.1.18}$$

corresponding to a_1 traversals of the first edge, then b_1 traversals of the second, then another a_2 of the first, and so on. Thus, as we see, $g_1 = g_2 = g$. The sum $\sum_{i=1}^{g} a_i$ is equal to s_1 and $\sum_{i=1}^{g} b_i = s_2$. In the general term in (3.1.17), $b(s_1, g)$ is the number of ways to decompose s_1 into a sum of a_i's, $b(s_2, g)$ is the number of ways to decompose s_2 into a sum of b_i's multiplied by the weight factor $(t/r)^{g_1+g_2-j}$ and divided by g, which corresponds to the cyclic symmetry and takes care of the repetitions at the same time (as will be explained in detail in the next section). There is no approximation involved in (3.1.17).

Taking the limit $B \to \infty$ of $D_{(s_1,s_2)}(B)$ termwise while keeping $q_1 = s_1/B$, $q_2 = s_2/B$ fixed, we obtain[2]

$$\begin{aligned} D(q_1, q_2) &= 1 + \frac{1}{2} q_1 q_2 2^2 + \frac{1}{3}\frac{1}{2!} q_1^2 \frac{1}{2!} q_2^2 2^4 + \ldots \\ &= \sum_{g=1}^{\infty} \frac{(4q_1q_2)^{g-1}}{g!(g-1)!} = \frac{I_1\left(4\sqrt{q_1q_2}\right)}{2\sqrt{q_1q_2}}, \end{aligned} \tag{3.1.19}$$

where $I_1(x)$ is a Bessel function, and so, using the substitution $q_1 = (\tau + \tau\cos\phi)/2$ we evaluate

$$\begin{aligned} H_2 &= \int_0^{\tau} \frac{I_1^2(4\sqrt{q_1(\tau - q_1)})}{4q_1(\tau - q_1)} dq_1 = \frac{1}{2\tau}\int_0^{\pi} \frac{I_1^2\left(2\tau\sin\phi\right)}{\sin\phi} d\phi \\ &= \frac{1}{4\tau^2}\left(I_1(4\tau) - 2\tau\right). \end{aligned} \tag{3.1.20}$$

Thus,

$$K_2(\tau) = 2\exp\left(-4\tau\right)\left(I_1(4\tau) - 2\tau\right). \tag{3.1.21}$$

Since $I_1(4\tau) = 2\tau + 4\tau^3 + O(\tau^5)$, $K_2(\tau)$ is of order τ^3 as $\tau \to 0$.

[2]In this particular case it is possible to justify the validity of the termwise limit: individual terms in $D_{(s_1,s_2)}(B)$ are increasing with B and the whole sum is bounded from above by$D(3\tau, 3\tau)$.

3.1.4 $K_j(\tau)$ for general j

We now proceed to calculate the degeneracy factor $D_{\mathbf{s}}(B)$ of (3.1.8) for general j. Without loss of generality we assume that the edges numbered 1 to j are traversed. We are looking for the number $N_{s_1,\dots,s_j}^{g_1,\dots,g_j}$ of all orbits which pass through the bond i s_i times in such a way that these traversals grouped into g_i groups.

Let us consider a slightly different problem. We want to count the number of all sequences of symbols, s_i symbols of the type i grouped into g_i groups. We require the sequences to start with a group of 1s and to end with a group of symbols different from 1. The difference from the orbits is that we *do not* identify the sequences obtained from one another by a shift. Each orbit $\mathbf{p}$ will then correspond to $g_1/r_{\mathbf{p}}$ such sequences which is best illustrated with an example.

Example 5. The orbit $(1,2,1,1,3,3,1,4)$ corresponds to $3/1 = 3$ sequences

$$[1,2,1,1,3,3,1,4],\ [1,1,3,3,1,4,1,2] \text{ and } [1,4,1,2,1,1,3,3]. \tag{3.1.22}$$

The orbit $(1,2,1,1,3,1,2,1,1,3)$ with $r_p = 2$ will correspond to $4/2 = 2$ sequences

$$[1,2,1,1,3,1,2,1,1,3] \text{ and } [1,1,3,1,2,1,1,3,1,2]. \tag{3.1.23}$$

Thus if we divide the number of all sequences, characterised by $s_1,\dots,s_j$ and $g_1,\dots,g_j$, by g_1 then we will obtain the number of all periodic orbits with the repetitions *already taken into account*. In fact, this is what was done in the previous section: we divided the number of all sequences, $b(s_1,g)b(s_2,g)$, by the number of groups $g_1 = g$.

To obtain all possible sequences we follow the following algorithm. First we divide the symbols i into g_i groups. Then we mix the groups in such a way that: (a) the order of the groups of the same symbol is preserved, (b) the first group of 1s comes first, (c) the last group is not a group of 1s and (d) no

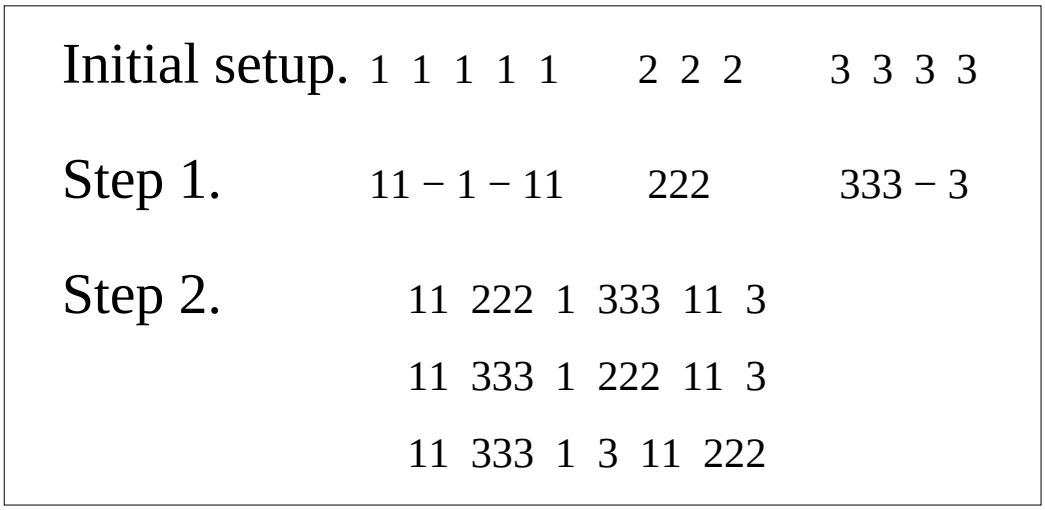

Figure 3.3: An example of producing sequences satisfying conditions (a)-(d) for $s_1 = 5$, $s_2 = 3$, $s_3 = 4$, $g_1 = 3$, $g_2 = 1$ and $g_3 = 2$.

two groups of the same symbols stand next to each other. This algorithm is illustrated in Fig. (3.3).

The number of possible sequences of the given structure is thus given by the product of the available choices at each step,

$$R_{g_1,\ldots,g_j} \prod_{i=1}^{j} \binom{s_i - 1}{g_i - 1}. \tag{3.1.24}$$

The first step produces the factors $b(s_i, g_i) = \binom{s_i-1}{g_i-1}$, where $b(s, g)$ is the number of decompositions of the integer s into a sum of g nonzero summands, see Section A.2. The second step gives the factor $R_{g_1,\ldots,g_j}$ which is the number of ways to mix $g_1, \ldots, g_j$ groups in such a way that conditions (a)-(d) are satisfied and which is discussed in detail in Section A.3. This factor, called the *number of permutation without liaisons* is equal to

$$R_{g_1,\ldots,g_j} = (-1)^G g_1 \sum_{k_1,\ldots,k_j} \frac{(-1)^{k_1+\ldots+k_j}}{k_1 + \ldots + k_j} \binom{k_1 + \ldots + k_j}{k_1, \ldots, k_j} \prod_{i=1}^{j} \binom{g_i - 1}{k_i - 1}, \tag{3.1.25}$$

Thus the number we are looking for, $N^{g_1,\ldots,g_j}_{s_1,\ldots,s_j}$, is given by

$$N^{g_1,\ldots,g_j}_{s_1,\ldots,s_j} = (-1)^G \sum_{k_1,\ldots,k_j} \frac{(-1)^K}{K} \binom{K}{k_1, \ldots, k_j} \prod_{i=1}^{j} \binom{g_i - 1}{k_i - 1} \binom{s_i - 1}{g_i - 1}, \tag{3.1.26}$$

where we denoted $K = k_1 + \ldots + k_j$.

Going back to $D_{\mathbf{s}}(B)$ we obtain with the aid of Eq. (3.1.26)

$$\begin{aligned} D_{\mathbf{s}}(B) &= \sum_{g_1=1}^{s_1} \cdots \sum_{g_j=1}^{s_j} N_{s_1,\ldots,s_j}^{g_1,\ldots,g_j} \left(\frac{t}{r}\right)^{G-j} \\ &= \sum_{g_1,\ldots,g_j} \left(-\frac{t}{r}\right)^{G-j} (-1)^j \sum_{k_1,\ldots,k_j} \frac{(-1)^K}{K} \binom{K}{k_1,\ldots,k_j} \\ &\qquad \times \prod_{i=1}^{j} \binom{g_i-1}{k_i-1} \binom{s_i-1}{g_i-1} \\ &= (-1)^j \sum_{g_1,\ldots,g_j} \sum_{k_1,\ldots,k_j} \frac{(-1)^K}{K} \binom{K}{k_1,\ldots,k_j} \\ &\qquad \times \prod_{i=1}^{j} \left(-\frac{t}{r}\right)^{g_i-1} \binom{g_i-1}{k_i-1} \binom{s_i-1}{g_i-1} \end{aligned} \tag{3.1.27}$$

where, as before, $G = \sum_{i=1}^{j} g_i$ and $K = \sum_{i=1}^{j} k_i$. Now we take the limit $B \to \infty$ termwise keeping $s_i/B = q_i$ fixed

$$\left(-\frac{t}{r}\right)^{g_i-1} \binom{s_i-1}{g_i-1} = \left(\frac{2}{B-2}\right)^{g_i-1} \binom{s_i-1}{g_i-1} \to \frac{(2q_i)^{g_i-1}}{(g_i-1)!}. \tag{3.1.28}$$

We obtain

$$D(q_1,\ldots,q_j) = \sum_{g_1,\ldots,g_j} \sum_{k_1,\ldots,k_j} \frac{(-1)^K}{K} \binom{K}{k_1,\ldots,k_j} \prod_{i=1}^{j} \frac{(2q_i)^{g_i-1}}{(g_i-1)!} \binom{g_i-1}{k_i-1}, \tag{3.1.29}$$

where the summation over g_i goes from 1 to infinity, k_i goes from 1 to g_i and we dropped the factor $(-1)^j$ because $D(q_1,\ldots,q_j)$ is going to be squared. Interchanging the summation signs and rearranging the general term in the product gives

$$\begin{aligned} D(q_1,\ldots,q_j) &= \sum_{k_1,\ldots,k_j} \sum_{g_1,\ldots,g_j} \frac{(-1)^K}{K} \binom{K}{k_1,\ldots,k_j} \prod_{i=1}^{j} \frac{(2q_i)^{g_i-k_i}}{(g_i-k_i)!} \frac{(2q_i)^{k_i-1}}{(k_i-1)!} \\ &= \sum_{k_1,\ldots,k_j} \frac{(-1)^K}{K} \binom{K}{k_1,\ldots,k_j} \prod_{i=1}^{j} \frac{(2q_i)^{k_i-1}}{(k_i-1)!} \sum_{g_1,\ldots,g_j} \prod_{i=1}^{j} \frac{(2q_i)^{g_i-k_i}}{(g_i-k_i)!}, \end{aligned} \tag{3.1.30}$$

where now the summation over k_i goes from 1 to infinity and g_i goes from k_i to infinity. Performing the summations over g_is we get $\prod_{i=1}^{j} \exp(2q_i)$ and, since

$q_1 + \ldots + q_j = \tau$ and $\exp(q_1 + \ldots + q_j) \approx \exp(q_1) + \ldots + \exp(q_j)$, we arrive at

$$D(q_1, \ldots, q_j) = \exp(2\tau) \sum_{k_1,\ldots,k_j} \frac{(-1)^K}{K} \binom{K}{k_1, \ldots, k_j} \prod_{i=1}^{j} \frac{(2q_i)^{k_i-1}}{(k_i-1)!}, \qquad (3.1.31)$$

where the summation over k_i goes from 1 to infinity.

For convenience we shift the summation, $n_i = k_i - 1$,

$$D(q_1, \ldots, q_j) = \exp(2\tau) \sum_{n_1,\ldots,n_j=0}^{\infty} (-2)^N (N+j-1)! \prod_{i=1}^{j} \frac{q_i^{n_i}}{n_i!(n_i+1)!}, \quad (3.1.32)$$

where $N = \sum_{i=1}^{j} n_i$. Using the fact once again that as $B \to \infty$ the summation in (3.1.10) can be replaced by the integral

$$H_j = \int_{\sum_{i=1}^{j} q_i = \tau} D^2(q_1, \ldots, q_j) dq_1 \ldots dq_{j-1}, \qquad (3.1.33)$$

where the integration is performed over $j-1$ variables. It is clear that to perform the integration we need to do the integrals of the type

$$\int_{\sum_{i=1}^{j} q_i = \tau} q_1^{m_1} \cdots q_j^{m_j} dq_1 \ldots dq_{j-1}. \qquad (3.1.34)$$

For completeness we include the derivation of this integral for $j = 3$. We have

$$\int_{q_1+q_2+q_3=\tau} q_1^{m_1} q_2^{m_2} q_3^{m_3} dq_1 dq_2 dq_3 = \int_0^{\tau} q_2^{m_2} dq_2 \int_0^{\tau-q_2} q_1^{m_1} (\tau - q_2 - q_1)^{m_3} dq_1. \qquad (3.1.35)$$

Thus first we need to evaluate the integral of the form

$$\int_0^y x^a (y-x)^b dx, \qquad (3.1.36)$$

which is exactly (3.1.34) for $j = 2$. Repeatedly integrating by parts we obtain

$$\begin{aligned} \int_0^y x^a (y-x)^b dx &= \frac{b}{a+1} \int_0^y x^{a+1} (y-x)^{b-1} dx = \ldots \\ \ldots &= \frac{b!}{(a+1)\cdots(a+b)} \int_0^y x^{a+b} dx \\ &= \frac{a!b!}{(a+b+1)!} y^{a+b+1}. \end{aligned} \qquad (3.1.37)$$

Substituting this result into Eq. (3.1.35) produces

$$\int_{q_1+q_2+q_3=\tau} q_1^{m_1} q_2^{m_2} q_3^{m_3} dq_1 dq_2 dq_3 = \frac{m_1! m_3!}{(m_1+m_3+1)!} \int_0^\tau q_2^{m_2} (\tau - q_2)^{m_1+m_3+1} dq_2$$
$$= \frac{m_1! m_3!}{(m_1+m_3+1)!} \frac{m_2!(m_1+m_3+1)!}{(m_1+m_2+m_3+1)!} \tau^{m_1+m_2+m_3}$$
$$= \frac{m_1! m_2! m_3!}{(m_1+m_2+m_3+1)!} \tau^{m_1+m_2+m_3}. \quad (3.1.38)$$

It is straightforward to derive the formula for general j,

$$\int_{\sum_{i=1}^j q_i = \tau} q_1^{m_1} \cdots q_j^{m_j} dq_1 \ldots dq_{j-1} = \frac{m_1! \cdots m_j!}{(M+j-1)!} \tau^{M+j-1}, \quad (3.1.39)$$

where $M = \sum_{i=1}^j m_i$.

Now we expand the square in Eq. (3.1.33) and apply Eq. (3.1.39) to obtain

$$H_j = \exp(4\tau) \sum_{\substack{k_1,\ldots,k_j=0 \\ n_1,\ldots,n_j=0}}^{\infty} (-2)^{N+K} \tau^{N+K+j-1} \frac{(N+j-1)!(K+j-1)!}{(N+K+j-1)!}$$
$$\times \prod_{i=1}^j \frac{(n_i+k_i)!}{n_i! k_i! (n_i+1)! (k_i+1)!}, \quad (3.1.40)$$

where $K = \sum_{i=1}^j k_i$ and $N = \sum_{i=1}^j n_i$. Therefore, the final result for $K_j(\tau)$ is

$$K_j(\tau) = \frac{4^j}{j!} \sum_{M=0}^{\infty} C_M \tau^{M+j+1} \quad (3.1.41)$$

and so

$$K^{lim}(\tau) = K_1(\tau) + \sum_{j=2}^{\infty} \sum_{M=0}^{\infty} \frac{4^j}{j!} C_M \tau^{M+j+1}, \quad (3.1.42)$$

where

$$C_M = (-2)^M \sum_{k_1+\ldots+k_j+n_1+\ldots+n_j=M} \frac{(K+j-1)!(N+j-1)!}{(M+j-1)!} \prod_{i=1}^j \frac{\binom{n_i+k_i}{n_i}}{(n_i+1)!(k_i+1)!} \quad (3.1.43)$$

with $K = \sum_{i=1}^j k_i$, $N = \sum_{i=1}^j n_i$, and the sum being performed over the $2j-1$ variables k_i and n_i (i.e. $2j$ variables minus one constraint).

This is the main result of the chapter. It constitutes a general formula for computing the coefficients in the expansion of $K(\tau)$ (from now on we will

always omit the overscrip *lim* when talking about $K^{lim}(\tau)$) in powers of τ around $\tau = 0$. Note that as $\tau \to 0$, the sum in (3.1.42) tends to zero as τ^3, and so it follows from (3.1.13) that $K(\tau) \to 1$ in this limit. This is the same as for the Poisson form factor, and unlike the random-matrix results, which all approach zero linearly in τ. However, the Poisson form factor is independent of τ, and $K(\tau)$ here clearly is not: after an initial decrease as τ increases, it eventually rises to the limiting value of one[11]. In this sense, the result is intermediate between the Poisson and random-matrix forms.

The expression for C_M can be written in another form that is more suitable for numerical computation. Defining

$$F_1(K,N) = \frac{\binom{K+N}{N}}{(N+1)!(K+1)!} \tag{3.1.44}$$

and using

$$\begin{aligned} &\sum_{k_1+\ldots+k_j+n_1+\ldots+n_j=M} \frac{(K+j-1)!(N+j-1)!}{(M+j-1)!} \prod_{i=1}^{j} \frac{\binom{n_i+k_i}{n_i}}{(n_i+1)!(k_i+1)!} \\ &= \sum_{K+N=M} \frac{(K+j-1)!(N+j-1)!}{(M+j-1)!} \sum_{\substack{k_1+\ldots+k_j=K \\ n_1+\ldots+n_j=N}} \prod_{i=1}^{j} \frac{\binom{n_i+k_i}{n_i}}{(n_i+1)!(k_i+1)!} \end{aligned} \tag{3.1.45}$$

it follows that

$$C_M = (-2)^M \sum_{K=0}^{M} \frac{(K+j-1)!(M-K+j-1)!}{(M+j-1)!} F_j(K, M-K), \tag{3.1.46}$$

where

$$F_j(K,N) = \sum_{k=0}^{K} \sum_{n=0}^{N} F_1(k,n) F_{j-1}(K-k, N-n), \tag{3.1.47}$$

which is a form of convolution. The expression (3.1.46) for the coefficients C_M is computationally more convenient because there is a clear recursive relation for the coefficients $F_j(K,N)$ which can be further facilitated using the discrete Fourier transform. The results of numerical computations with the first few coefficients of the expansion are shown in Fig. 3.4. Even few first terms of the expansion give a reasonable agreement with the numerical data up to around

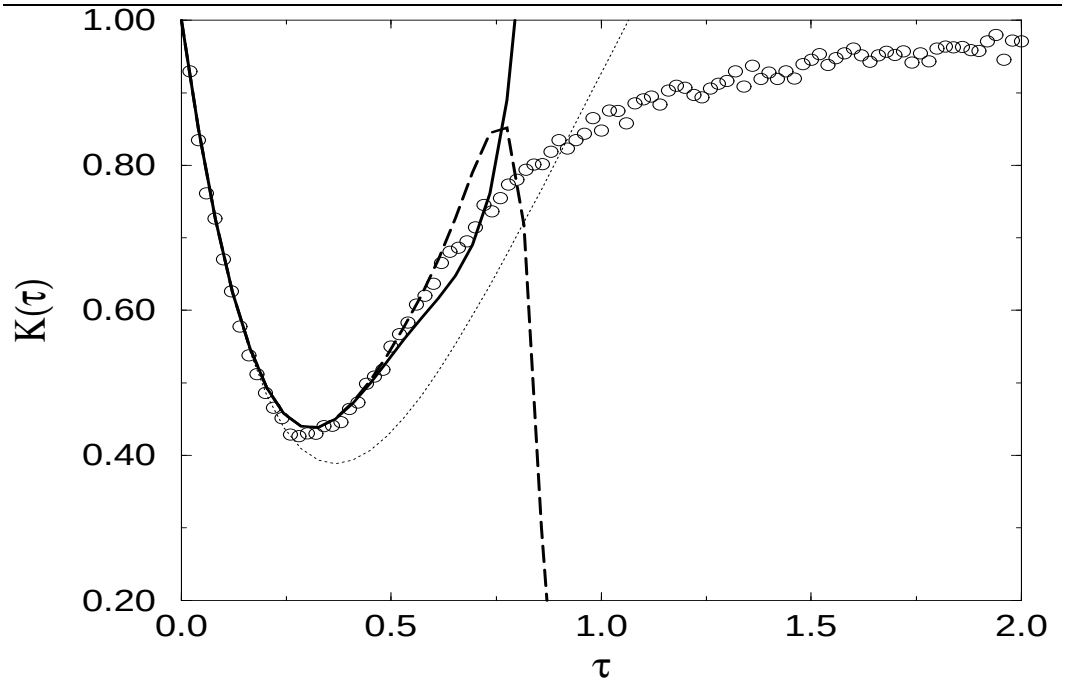

Figure 3.4: The first 11 terms (solid line) and the first 7 terms (dashed line) in the expansion for $K(\tau)$, compared with data from the numerical simulation by Kottos and Smilansky [20] for $\langle|\mathrm{Tr}\mathbf{S}^{2k}|^2\rangle/(4B)$, $B = 50$ (circles). The dotted line corresponds to the diagonal approximation (3.2.3)

0.6. However it seems that after 0.6 the series might diverge. In Section 3.3 we will see that it is indeed the case and we will study the possible ways to improve the convergence.

3.2 A summable approximation

One possible approximation to $\widetilde{K}(\tau)$ can be made by ignoring two contributions:

1. the off-diagonal terms in (3.1.1). We call a term in the summation in (3.1.1) diagonal if it corresponds to $\mathbf{p} = \mathbf{q}$, otherwise we call it off-diagonal. In symbolic form, the diagonal approximation is

$$K(\tau) \approx K^{diag}(\tau) = \frac{1}{L^2} \sum_{n=2}^{\infty} \sum_{\mathbf{p} \in \mathcal{P}_n} \left(\frac{l_{\mathbf{p}}}{r_{\mathbf{p}}} \right)^2 A_{\mathbf{p}}^2 \delta \left(\tau - \frac{l_{\mathbf{p}}}{L} \right). \qquad (3.2.1)$$

2. all orbits for which the number of backscatterings is less than the maximum in their degeneracy class or, in other terms, orbits which have a g_i greater than one. For example, the orbits (1,1,4,6,6,6) and (1,1,6,4,6,6) belong to the same degeneracy class. The first orbit gives the contribution of t^3r^3 which, in the limit $B \to \infty$ is more substantial than the second orbit's contribution of t^4r^2. It is not hard to see that out of each degeneracy class only $(j-1)!$ orbits will survive this approximation, where j, as before, is the number of distinct edges traversed by the orbit.

The result of the above approximations is that the contribution E_j of the degeneracy classes in (3.1.9) is reduced to a factor of $(j-1)!$, the contribution of one degeneracy class, multiplied by the number of degeneracy classes, $\binom{k-1}{j-1}$:

$$K^{diag}(\tau) \approx K_1(\tau) + \lim_{B\to\infty} \frac{(2k)^2 B}{L^2} \sum_{j=2}^{\infty} \binom{B}{j} \left(\frac{2}{B}\right)^{2j} \left(\frac{B-2}{B}\right)^{2k-2j} (j-1)! \binom{k-1}{j-1}. \quad (3.2.2)$$

Taking the limit $B \to \infty$ termwise, with $\tau = k/B$ fixed, we arrive at

$$\begin{aligned} K^{diag}(\tau) &\approx K_1(\tau) + \tau^2 \sum_{j=2}^{\infty} 2^{2j} \exp(-4\tau) \frac{\tau^{j-1}}{j!} \\ &= \exp(-4\tau) + \tau \exp(-4\tau) \sum_{j=2}^{\infty} \frac{(4\tau)^j}{j!} \\ &= \exp(-4\tau) + \tau \exp(-4\tau)(\exp(4\tau) - 1 - 4\tau) \\ &= \tau + \exp(-4\tau)(1 - \tau - 4\tau^2), \end{aligned} \quad (3.2.3)$$

which, in the limit of large B with $\tau = k/B$ fixed, is exactly equal to an approximation to $\langle |\mathrm{Tr}\mathbf{S}^{2k}|^2 \rangle/(4B)$ obtained in [20] using a different approach detailed below. Interestingly, the first four terms in the expansion of K^{diag} in powers of τ agree with those of K computed in the last section. The rest do not.

It is worth remarking that one can get exactly the same asymptotic formula for $K^{diag}(\tau)$ using only assumption 1. Following [20], we obtain from (3.2.1)

$(n = 2k)$

$$\begin{aligned} K^{diag}(\tau) &= \lim_{B\to\infty} \frac{4kB}{L^2} \sum_{\mathbf{p}\in\mathcal{P}_{2k}} \frac{k}{r_{\mathbf{p}}^2} A_{\mathbf{p}}^2 \qquad (3.2.4) \\ &= K_1(\tau) + \lim_{B\to\infty} \frac{4kB}{L^2} \left(\sum_{\mathbf{p}\in\mathcal{P}_{2k}} \frac{k}{r_{\mathbf{p}}^2} A_{\mathbf{p}}^2 - B \left(\frac{B-2}{B}\right)^{2k} \right) \\ &\approx K_1(\tau) + \lim_{B\to\infty} \frac{4kB}{L^2} \left(\sum_{\mathbf{p}\in\mathcal{P}_{2k}} \frac{k}{r_{\mathbf{p}}} A_{\mathbf{p}}^2 - B \left(\frac{B-2}{B}\right)^{2k} \right), \end{aligned}$$

where in the second line we have split $K^{diag}(\tau)$ into $K_1(\tau)$ and "the rest", as before. The only difference between the second and the third line is in the power of $r_{\mathbf{p}}$, i.e. in the third line we partly ignored the repetitions. We can do that since the orbits without the repetitions are exponentially dominant (it can be explicitly shown using Möbius inversion theorem). But to do it we first have to separate a special class of orbits, the one restricted to one edge, out of the sum.

Now we are going to evaluate "the rest" using a sum rule. We note that $\sum_{p\in\mathcal{P}_{2k}} \frac{k}{r_p} A_{\mathbf{p}}^2 = \mathrm{Tr}\mathbf{A}^k$, where the $B \times B$ matrix $\mathbf{A}$ is given by

$$A_{b_1,b_2} = \left(\frac{2}{B} - \delta_{b_1,b_2}\right)^2, \qquad (3.2.5)$$

where b_1 and b_2 are nondirected bonds. To evaluate the trace of any power of the matrix $\mathbf{A}$ we need to know its eigenvalues. First of all, 1 is an eigenvalue which corresponds to the eigenvector consisting of all ones: the sum of elements in any row of the matrix $\mathbf{A}$ is $(2/B-1)^2 + 4(B-1)/B^2 = 1$. Let us now consider the eigenvalue equation for $B = 3$

$$\begin{aligned} \begin{vmatrix} \frac{1}{9}-\lambda & \frac{4}{9} & \frac{4}{9} \\ \frac{4}{9} & \frac{1}{9}-\lambda & \frac{4}{9} \\ \frac{4}{9} & \frac{4}{9} & \frac{1}{9}-\lambda \end{vmatrix} &= \begin{vmatrix} \frac{1}{9}-\lambda & \frac{4}{9} & \frac{4}{9} \\ \frac{3}{9}+\lambda & -\frac{3}{9}-\lambda & 0 \\ \frac{3}{9}+\lambda & 0 & -\frac{3}{9}-\lambda \end{vmatrix} \\ &= (3/9+\lambda)^2 \begin{vmatrix} \frac{1}{9}-\lambda & \frac{4}{9} & \frac{4}{9} \\ 1 & -1 & 0 \\ 1 & 0 & -1 \end{vmatrix} = 0, \qquad (3.2.6) \end{aligned}$$

where the first line was subtracted from the rest and then the common factor $(3/9+\lambda)^2$ was separated. From here it is obvious that $3/9$ is an eigenvalue with multiplicity 2. For general B the factor to separate would be of the form $2/B^2-(2/B-1)^2+\lambda$ of the multiplicity $B-1$. Thus the matrix $\mathbf{A}$ has the eigenvalues $\{1,\frac{B-4}{B},\ldots,\frac{B-4}{B}\}$ and, therefore,

$$\mathrm{Tr}\mathbf{A}^k = 1+(B-1)\left(\frac{B-4}{B}\right)^k. \tag{3.2.7}$$

Using this we write

$$\begin{aligned} K^{diag}(\tau) \approx & K_1(\tau)+\lim_{B\to\infty}\tau\left(1+(B-1)\left(\frac{B-4}{B}\right)^k - B\left(\frac{B-2}{B}\right)^{2k}\right) \\ =& K_1(\tau)+\lim_{B\to\infty}\tau\left(1-\left(\frac{B-4}{B}\right)^k + B\left\{\left(\frac{B-4}{B}\right)^k-\left(\frac{B-2}{B}\right)^{2k}\right\}\right) \\ =& \exp(-4\tau)+\tau\left(1-\exp(-4\tau)-4\tau\exp(-4\tau)\right), \end{aligned} \tag{3.2.8}$$

where we have used the limit

$$\lim_{n\to\infty} n\left(\left(1+\frac{1}{an}+\frac{1}{(an)^2}\right)^n-\left(1+\frac{1}{an}\right)^n\right)=\frac{e^{1/a}}{a}. \tag{3.2.9}$$

We note that Eq.(3.2.8) is exactly the same as Eq. (3.2.3). This means that the orbits ignored in the second assumption above do not contribute to the diagonal approximation in the limit $B\to\infty$. The fact that they do contribute to the full expansion of $K(\tau)$ shows the limitations of the diagonal approximation.

3.3 Numerical analysis of the series expansion

Before we actually proceed to analyse the power series (3.1.41)-(3.1.43) numerically, we would like to prove that there is an interval on which the series converge.

Proposition 4. *The radius of convergence of the series (3.1.41)-(3.1.43) is greater than zero.*

Proof. Let us first find an upper bound on the modulus of the coefficient C_M defined in Eq. (3.1.41). Starting off with Eq. (3.1.46) we write

$$\begin{aligned} |C_M| &\leq M2^M \max_{K+N=M} \frac{(K+j-1)!(N+j-1)!}{(M+j-1)!} F_j(K,N) \\ &\leq M2^M (j-1)! \max_{K+N=M} F_j(K,N), \end{aligned} \tag{3.3.1}$$

where we used the fact that (assuming, without loss of generality, that $K \geq N$)

$$\begin{aligned} &(K+j-1)!(N+j-1)! \leq (K+j)!(N+j-2)! \\ &\quad \leq (K+j+1)!(N+j-3)! \leq \ldots \leq (K+N+j-1)!(j-1)! \end{aligned} \tag{3.3.2}$$

and thus

$$\max_{K+N=M} \frac{(K+j-1)!(N+j-1)!}{(M+j-1)!} = (j-1)!. \tag{3.3.3}$$

To find the maximum of the factor $F_j(K,N)$ we estimate

$$F_j(K,N) \leq \sum_{K,N} F_j(K,N), \tag{3.3.4}$$

and apply the recursion relation (3.1.47) to obtain

$$\begin{aligned} \sum_{K,N} F_j(K,N) &= \sum_{K=0}^{\infty}\sum_{N=0}^{\infty}\sum_{k=0}^{K}\sum_{n=0}^{N} F_1(k,n) F_{j-1}(K-k,N-n) \\ &= \sum_{k,n,r,s} F_1(k,n) F_{j-1}(r,s) = \sum_{k,n} F_1(k,n) \sum_{k,n} F_{j-1}(k,n) = F^j, \end{aligned} \tag{3.3.5}$$

where

$$F = \sum_{k,n} F_1(k,n) = \sum_{k,n} \frac{(k+n)!}{k!n!(k+1)!(n+1)!} < \infty. \tag{3.3.6}$$

Thus

$$|C_M| \leq M2^M (j-1)! F^j, \tag{3.3.7}$$

and substituting it into Eq. (3.1.42) we obtain

$$|K(\tau)| < K_1(\tau) + \tau \sum_{M=0}^{\infty} M2^M \tau^M \times \sum_{j=2}^{\infty} \frac{(4F\tau)^j}{j}, \tag{3.3.8}$$

which implies that the radius of convergence is greater or equal to $(4F)^{-1}$. □

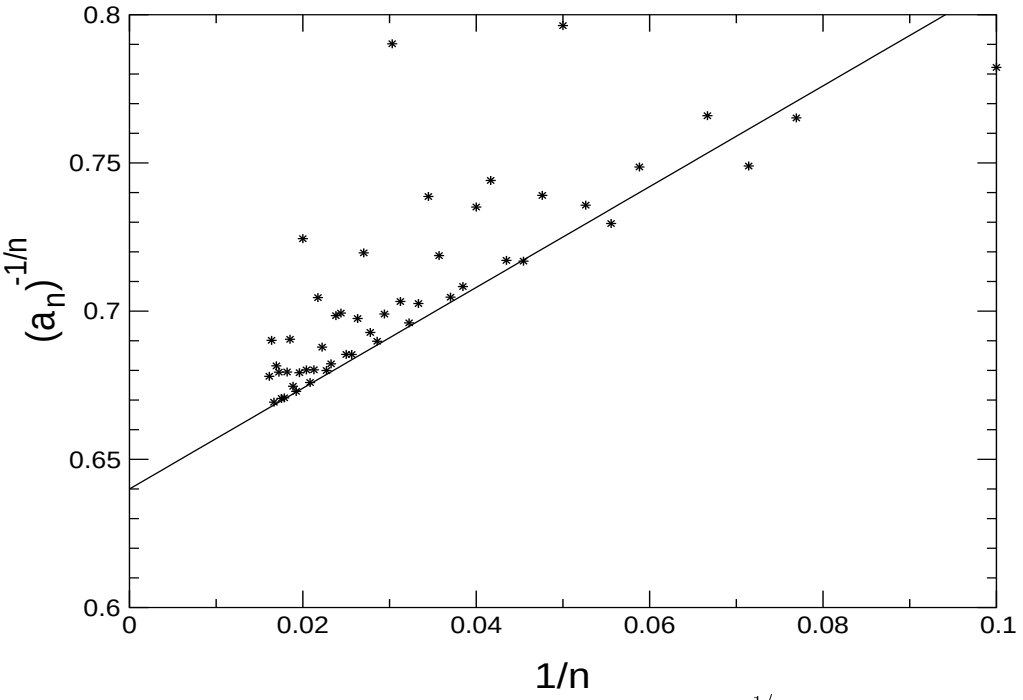

Figure 3.5: Determining the radius of convergence: $(a_n)^{-1/n}$ is plotted against $1/n$. The radius of convergence is the lower limit of the plotted points as $1/n \to 0$. The line is to guide the eye only.

Remark 3. The bound found above, $(4F)^{-1} \approx 0.061$, is very far from being exact, but the effort needed to derive a better one is, at the current stage, exponentially greater than the importance of having an exact result.

The expressions for the coefficients of expansion of $K(\tau)$, Eqs. (3.1.46)-(3.1.47), provide us with a clear numerical recipe for their computation and, given enough computer resources, one can compute as many of the coefficients as needed to get a fair idea of what the behaviour of the expansion is like. The coefficients can be computed exactly, in the rational form.

Let us write

$$K(\tau) = \exp(-4\tau) + \sum_{i=3}^{\infty} a_i \tau^i. \tag{3.3.9}$$

In our numerical study we computed coefficients up to a_{60}. First of all we can estimate the radius of convergence of the series by plotting the numbers a_n/a_{n+1} or the numbers $(a_n)^{-1/n}$ as a function of n. In our case we have oscillating coefficients with increasing amplitude of the oscillations thus the

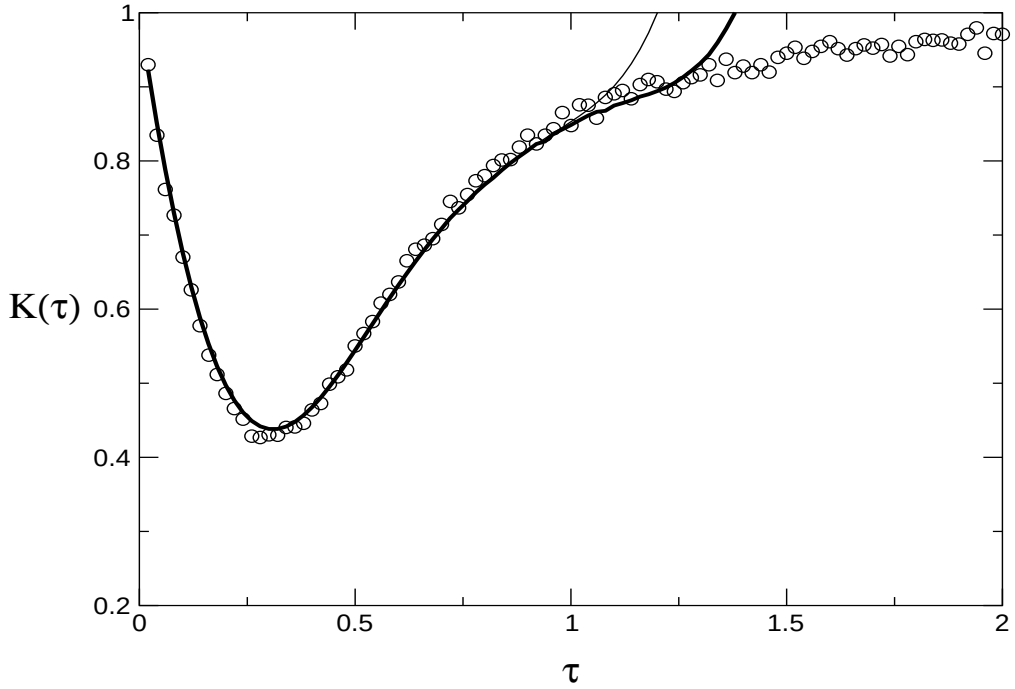

Figure 3.6: The result of Padé approximation of order $M = N - 1 = 21$ (thin line) and $M = N = 23$ (thick line) compared to the results of numerical computation of $K(\tau)$ [Kottos and Smilansky]. The approximation is good far beyond the radius of convergence (≈ 0.64).

better quantity to look at is the second one. Looking at the plot, Fig. 3.5, and estimating where the intersection with the y-axis would be, we can see that the radius of convergence is approximately 0.64. Before we continue analysing the coefficients of the series, let us try to approximate the form factor $K(\tau)$ by rational functions.

In other words, we are going to apply Padé approximation (see, for example, [30]) to the partial series we have. The general idea behind Padé approximation is the following. Let $S_K(x)$ be the K-th partial sum of the power series for some function $S(x)$,

$$S_K = \sum_{i=0}^{K} a_i x^i. \tag{3.3.10}$$

We are trying to represent $S(x)$ as a ratio of two polynomials $P_N(x)$ and $Q_M(x)$, of order N and M correspondingly,

$$S(x) = \frac{P_N(x)}{Q_M(x)} + o\big(x^{M+N}\big)\,, \qquad \text{as } x \to 0. \tag{3.3.11}$$

where by $o\left(x^{M+N}\right)$ we understand the terms of order higher than $M+N$. Rewriting Eq. (3.3.11) as

$$P_N(x) - Q_M(x)S(x) = o\left(x^{M+N}\right) \tag{3.3.12}$$

we obtain $M+N+1$ linear equations — the first $N+M+1$ coefficients of the series on the left are equal to zero. There are $M+N+2$ unknowns, the coefficients of P_N and Q_M, but since we are looking at the ratio P/Q, we can fix one of the coefficients, say put $Q_M(0)=1$. In fact, to solve Eq. (3.3.12) we do not need the whole of the series $S(x)$, the partial sum S_{M+N} is enough.

As an example we consider the $N=M=1$ approximation to our form factor. It is convenient to take the factor τ^3 out:

$$K(\tau) = \exp(-4\tau) + \tau^3\left(8 - \frac{32}{3}\tau + \frac{16}{3}\tau^2 + o(\tau^2)\right). \tag{3.3.13}$$

Then the equation for the coefficients of Q and P is taking the form

$$p_0 + p_1\tau - (1+q_1\tau)\left(8 - \frac{32}{3}\tau + \frac{16}{3}\tau^2\right) = o(\tau^2), \tag{3.3.14}$$

therefore

$$p_0 - 8 = 0, \qquad p_1 - 8q_1 + \frac{32}{3} = 0, \qquad \frac{32}{3}q_1 - \frac{16}{3} = 0, \tag{3.3.15}$$

which leads to

$$P_1(\tau) = 8 - \frac{20}{3}\tau, \qquad Q_1(\tau) = 1 + \frac{1}{2}\tau. \tag{3.3.16}$$

Very often the approximation $P_N(x)/Q_M(x)$ happens to be very good even beyond the radius of convergence. To understand it heuristically, suppose $S(x)$ is an expansion of a function which has a pole at the distance R from the origin somewhere in the complex plane, but not on the positive real line and we want to plot $S(x)$ for real $x>0$. If lucky, the pole of $S(x)$ will be represented by a zero of the polynomial $Q_M(x)$ and then the divergence of the original series will be absorbed into the rational function $P_N(x)/Q_M(x)$ while the remaining part $o\left(x^{M+N}\right)$ will be convergent and small. Then the approximating function

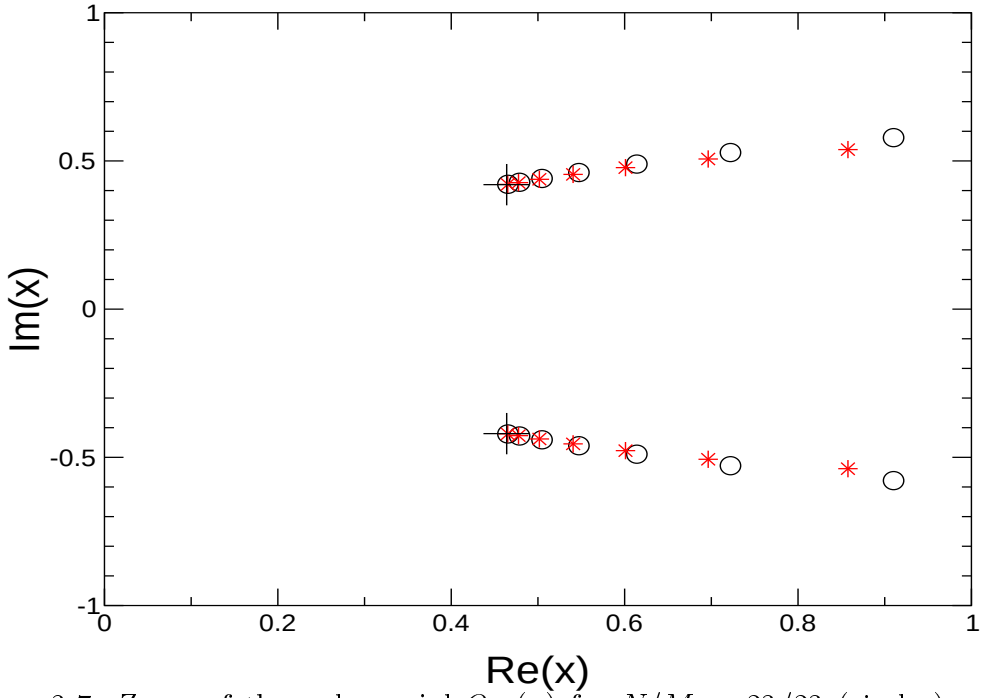

Figure 3.7: Zeros of the polynomial $Q_M(x)$ for $N/M = 23/23$ (circles) and $N/M = 24/23$ (stars). Only the poles nearest to the origin are shown on the plot. The conjectured positions of the singularities are marked by the crosses.

$P_N(x)/Q_M(x)$ will follow $S(x)$ closely even for the values of x greater than R. However most often it is not possible to say whether Padé approximation is going to work on a particular series before one actually tries it.

For our series the approximation happens to work best when $M = N$ or $M = N - 1$ with two examples plotted on Fig. 3.6. From comparison with the numerical data it is clear that Padé approximation extends the convergence of the series beyond the estimated radius of 0.64. The results for other choices of M and N are not very different as long as $|M - N|$ is not too large.

As mentioned earlier, one of the properties of Padé method is that the approximants P/Q try to represent the singularities of the original series with the poles, i.e. zeroes of the polynomial $Q(x)$. Some of the zeroes will not correspond to any properties of the approximated function, these "spurious" zeroes usually disappear or change their position when we change the order N of the approximating polynomials $P(x)$ and $Q(x)$. Those zeroes which persist when we change N are likely to correspond to the real singularities of $S(x)$.

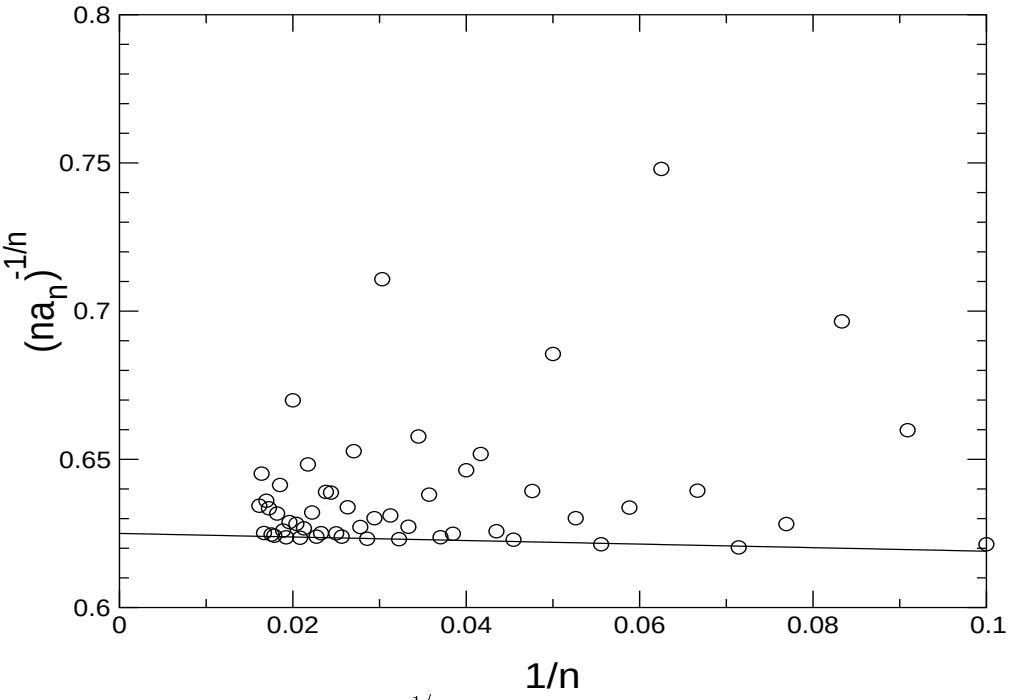

Figure 3.8: The quantity $(na_n)^{-1/n}$ is plotted against $1/n$. Again, the radius of convergence is given by the lower limit of the data as $1/n \to 0$. The line is to guide the eye only.

If a singularity of $S(x)$ is not a pole, it is often represented by a sequence of poles of the approximant. Looking at the pattern of the zeroes of the polynomial $Q(x)$ in our case, Fig. 3.7 we can see that there are two sequences converging approximately to $z = 0.464 + 0.42i$ and $\overline{z} = 0.464 - 0.42i$. This sequence is persistent and contains more zeroes larger N we take. This is a strong indication that z corresponds to an essential singularity of $K(\tau)$, the one which limits the convergence of the series, since $|z| \approx 0.626$.

Let us now go back to the coefficients of the expansion of $K(\tau)$. It is not unnatural to assume that the singularity at z is logarithmic. This would mean that the coefficients are well approximated by the formula $a_n = \Re\,(z^n/n)$. To check it we plot the quantity $(na_n)^{-1/n}$ against $1/n$, see Fig. 3.8. Indeed, the convergence now is much more "linear" than on Fig. 3.5. The estimated radius of convergence is now 0.625.

The further support to the claim that $a_n = \Re\,(z^n/n)$ will be presented in Chapter 5.

Chapter 4

Quantum return probability for trees

In this chapter we discuss an analogue of the form-factor for infinite trees, the quantum return probability. The work on trees was inspired by the paper by Schanz and Smilansky [21] who performed the analysis in the case of infinite chain (valency of every vertex is 2). We follow their work closely and derive the recursion relation for the return probability for a general infinite regular tree. Our main result is a general formula for the local contribution of a degeneracy class. This made possible a numerical investigation, since the complexity of the formulae do not encourage attempts to analyse the limiting behaviour of the return probability analytically. We also show a way to obtain a power series expansion of the return probability in the limit of large branching.

4.1 Definitions

We have defined tree is a connected graph without any cycles. We here consider mainly a special type of trees, the infinite one-sided regular tree, although most of the results can be easily extended to any trees.

An example of infinite one-sided regular tree is shown on Fig. 4.1. The one-sided tree has an origin, the vertex O of valency 1. All other vertices have

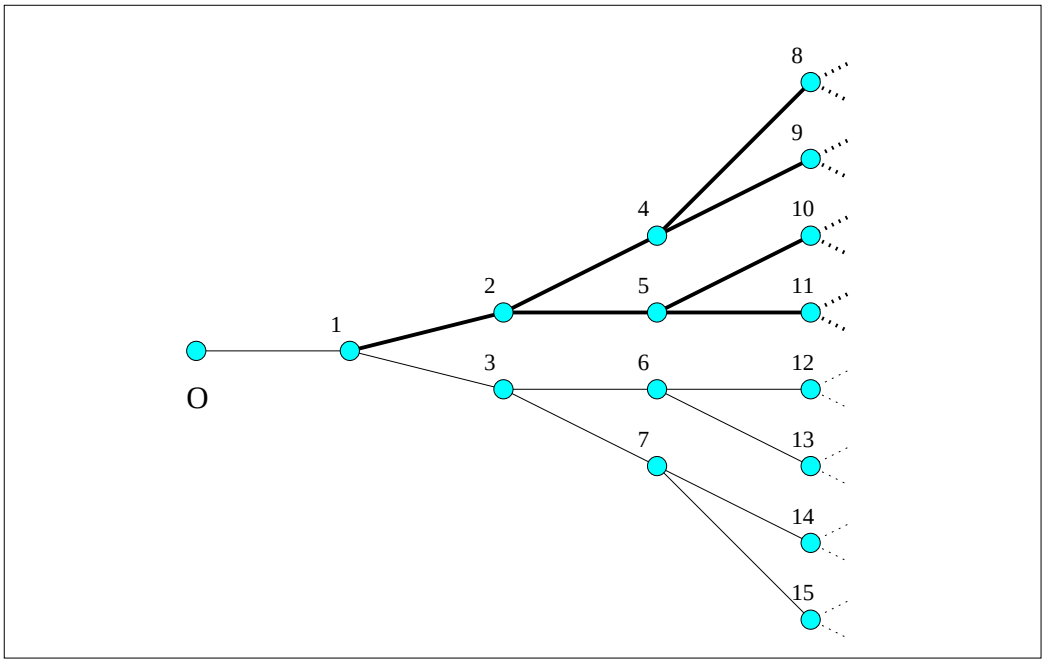

Figure 4.1: The one-sided infinite tree with $B = 3$. The upper subtree is shown with the thicker lines.

the same valency[1] B; B is equal to 3 for the graph on Fig. 4.1.

As described in Section 2.4, we associate a unitary matrix $\mathbf{S}^{(v)}$ to each vertex v of the infinite tree. To simplify matters we require that the matrices have the form

$$\mathbf{S}^{(v)} = \begin{pmatrix} r_v & t_v & \dots & t_v \\ t_v & r_v & \dots & t_v \\ \vdots & \vdots & \ddots & \vdots \\ t_v & t_v & \dots & r_v \end{pmatrix}, \tag{4.1.1}$$

i.e. all diagonal elements are equal to r_v while the non-diagonal elements are equal to t_v. Thus we have two types of "amplitudes": the amplitude r_v associated to the reflection (going from a bond b to the bond $\overline{b}$) and the amplitude t_v associated to the transmission. The matrix $\mathbf{S}_O$ corresponding to the origin is 1×1 and we fix $r_O = 1$.

The *quantum return probability* (also called the survival probability), which gives the probability to find the quantum particle at time t in its initial state

[1]Since the tree is infinite, the number of bonds is infinite thus we re-use B to denote the branching of the tree. However its role is very similar to the role of B for the star graphs.

ψ_0, taken from the corresponding Hilbert space, is given by

$$\left|\langle\psi_0|\mathbf{U}^t|\psi_0\rangle\right|^2, \tag{4.1.2}$$

where $\mathbf{U}$ is the time evolution operator. Its Cesàro average

$$\frac{1}{T}\int_0^T \left|\langle\psi_0|\mathbf{U}^t|\psi_0\rangle\right|^2 dt, \tag{4.1.3}$$

is called the *mean return probability over time* T. In our case (see Section 2.4) the evolution is discrete and the evolution operator is the matrix $\mathbf{DS}$, now of infinite size; the state vector ψ is the ℓ^2 vector of the amplitudes $A_{(i,j)}$ of the wave travelling from vertex i to vertex j. Thus the mean return probability in our case is given by

$$\frac{1}{N}\sum_{n=1}^{N}\left|\langle\psi_0|\left(\mathbf{DS}\right)^n|\psi_0\rangle\right|^2 \equiv \frac{1}{N}\sum_{n=1}^{N} P_B(n), \tag{4.1.4}$$

where by $P_B(n)$ we denoted the quantum return probability (not mean).

We will take ψ_0 to be the wave leaving the vertex O in the direction 11, i.e. we take the component $A_{(O,1)} = 1$ and $A_{(i,j)} = 0$ for all other choices of the vertices i and j. Then one can expand

$$\begin{aligned} P_B(n) &= \left|\langle\psi_0|\left(\mathbf{D}(k)\mathbf{S}\right)^n|\psi_0\rangle\right|^2 \\ &= \left|\sum_{[i_1=(O,1),i_2,\ldots,i_n]} \left(\mathbf{D}(k)\mathbf{S}\right)_{i_1,i_2}\left(\mathbf{D}(k)\mathbf{S}\right)_{i_2,i_3}\cdots\left(\mathbf{D}(k)\mathbf{S}\right)_{i_n,i_1}\right|^2 \\ &= \left|\sum_{\mathbf{p}\in\widetilde{\mathcal{P}_n}(O)} A_{\mathbf{p}}e^{ikl_{\mathbf{p}}}\right|^2, \end{aligned} \tag{4.1.5}$$

where the second sum is taken over all periodic sequences of bonds (see (2.1.5) and subsequent explanations) which start from the vertex O. The factor $A_{\mathbf{p}}$ is, as usual, the product of the elements of the matrix $\mathbf{S}$ over the sequence $\mathbf{p}$. We remind that the sequences are not identified with respect to the shift, in the sense that, for example, $[1,2,3,1,4]$ and $[1,4,1,2,3]$ are different sequences, unlike the situation we had with the orbits from $\mathcal{P}$.

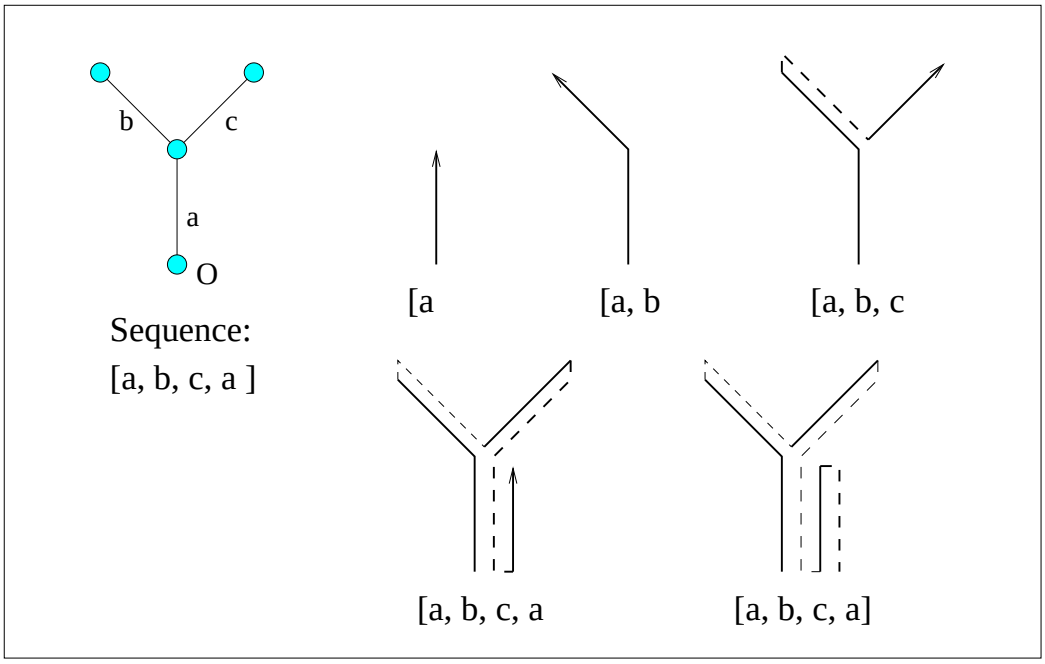

Figure 4.2: Step-by-step reconstruction of the sequence denoted by $[a, b, c, a]$. In the top left corner the subtree covered by the sequence is drawn (the bonds are relabelled for convenience). The bonds which are missed in the shortened notation are shown in dashed lines.

Due to the special structure of the tree all periodic sequences have even period. If a sequence left a vertex v along the bond $b = (v, v')$, it will later come back to v along the bond $\overline{b} = (v', v)$ and *not* along any other bond. This fact is crucial to our derivation and is specific to the trees. It is easy to see that when writing the code for a sequence on the tree, we can mention only the traversal of a bond in the *outward* direction; basing on this information we can always reconstruct the whole description of the orbit, see Fig. 4.2. Also, when we write the vector $\mathbf{s}$ for a degeneracy class, the element s_b (the staying rate on the bond b) counts the number of traversals of the bond b in *outward* direction only. The vectors $\mathbf{s}$ are now infinite dimensional but they have only finite number of nonzero components since we demand $|s| = \sum_b s_b = M$.

We now return to our definition of the quantum return probability. To the operations performed in Eq. (4.1.2) we add an averaging, either over a range of k or over individual lengths of the bonds of the tree G. It is easy to see that squaring the expression on the right-hand side of Eq. (4.1.5) and then applying

the averaging will lead to the expression for the quantum return probability after n steps,

$$P_B(n) = \sum_{\mathbf{p},\mathbf{q}\in\widetilde{\mathcal{P}_n}(O)} A_{\mathbf{p}}\overline{A_{\mathbf{q}}}\delta_{l_{\mathbf{p}},l_{\mathbf{q}}}, \tag{4.1.6}$$

where $\delta_{l_{\mathbf{p}},l_{\mathbf{q}}}$ is, as before, equal to 1 if $l_{\mathbf{p}} = l_{\mathbf{q}}$ and is 0 otherwise. Since all periodic sequences on a tree have even period, we put $n = 2M$. Rewriting Eq. (4.1.6) in the terms of degeneracy classes we arrive to the expression which we will use as the definition.

Definition 8. The *quantum return probability after* $2M$ *steps* is defined by

$$P_B(2M) = \sum_{\mathbf{s}:\ |\mathbf{s}|=M} \left| \sum_{\mathbf{p}:\ s(\mathbf{p})=\mathbf{s}} A_{\mathbf{p}} \right|^2, \tag{4.1.7}$$

where the sum is over all degeneracy classes of the sequences that start from the vertex O.

Besides being an interesting quantity in its own right, the quantum return probability is closely related to the existence of localised eigenstates of the evolution operator **DS**. Such states correspond to the pure point spectrum of **DS**. Since the underlying graph is no longer compact, the spectrum of **DS** can now contain both pure point and continuous (including singular continuous) parts. To see whether there is a pure point component we formally substitute the spectral decomposition

$$\mathbf{DS} = \int |\alpha\rangle e^{iE_\alpha}\langle\alpha| dE_\alpha \tag{4.1.8}$$

into the definition of the mean return probability

$$\begin{aligned}\lim_{N\to\infty}\frac{1}{N}\sum_{n=1}^{N} P_B(n) &= \lim_{N\to\infty}\frac{1}{N}\sum_{n=1}^{N}\left|\int e^{iE_\alpha}\left|\langle\psi|\alpha\rangle\right|^2 dE_\alpha\right|^2 \\ &= \iint \lim_{N\to\infty}\frac{1}{N}\sum_{n=1}^{N} e^{in(E_\alpha - E_{\alpha'})}\left|\langle\psi|\alpha\rangle\right|^2\left|\langle\psi|\alpha'\rangle\right|^2 dE_\alpha dE_{\alpha'} \\ &= \iint \left|\langle\psi|\alpha\rangle\right|^4 \delta_{E_\alpha,E_{\alpha'}} dE_\alpha dE_{\alpha'},\end{aligned} \tag{4.1.9}$$

where we used the identity

$$\lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} e^{inE} = \delta_{E,0}. \tag{4.1.10}$$

It is not hard to see that the last integral in Eq. (4.1.9) is equal to zero if the measure dE_α has only continuous part (for more rigorous statements and results we refer to [36]). Thus a nonzero limit of the mean return probability would signify the presence of the pure point spectrum, hence the localised states.

This was exactly the situation revealed by Schanz and Smilansky in [21] for the infinite chain graphs (an infinite chain is a tree with $B = 2$). It was found that the quantum return probability saturates to a finite value while its diagonal approximation decays diffusively. Thus the coherent (i.e. taking care of the degeneracy classes) summation of the contributions of different orbits really makes a difference. The aim of the following sections is to use the ideas from the previous Chapter to treat the contributions of the degeneracy classes in an exact way for $B > 2$.

But before doing so we give a brief summary of the related research. The localised eigenstates of the discrete Hamiltonian on infinite trees (called *Bethe lattice* in the literature) is a much studied topic, first introduced by Anderson [37]. We refer to the paper by Klein[38] for a review of the results in this area. Our model, however, is one step removed from the specification of the Hamiltonian. Instead, we start with the time evolution operator. In this respect our model is similar to the one considered by Chalker and Siak in [31], although in the model of [31] there is no time-reversal symmetry. Among other results, Chalker and Siak report the existence of normalizable localised states for a certain range of the parameter of the model.

For our model we also find a strong numerical evidence that the quantum return probability tends to a nonzero limit for certain values of the parameter. This implies that the mean return probability also tends to the same limit and, therefore, there are localised eigenstates. We also find that the transi-

tion between delocalisation and localisation occurs approximately at the same parameter value as in [31].

4.2 Recursion for the return probability

Consider the contribution $\sum_{\mathbf{p}:\, s(\mathbf{p})=\mathbf{s}} A_{\mathbf{p}}$ from one degeneracy class $\mathbf{s}$. For a given vertex v we define $m_1(v)$ to be the staying rate on the bond leading to v from the direction of the origin. We also denote by $m_2(v)$ the staying rate on the first bond leading out of v and so on up to $m_B(v)$, thus $m_1(v), \ldots, m_B(v)$ provide the local information about the bond staying rates around the vertex v. It turns out that the contribution of the degeneracy class $\mathbf{s}$ can be decomposed into a product,

$$\sum_{\mathbf{p}:\, s(\mathbf{p})=\mathbf{s}} A_{\mathbf{p}} = \prod_{v\in G} \mathcal{U}_v\Big(m_1(v), m_2(v), \ldots, m_B(v)\Big), \tag{4.2.1}$$

where the factor $\mathcal{U}_v\Big(m_1(v), m_2(v), \ldots, m_B(v)\Big)$ is the *local contribution of the degeneracy class* $\mathbf{s}$ which depends only on the matrix $\mathbf{S}^{(v)}$ and the local information about the degeneracy class, the numbers $m_1(v)$, ... ,$m_B(v)$. To explain why this happens we consider an example.

In the top left corner of Fig. 4.3 the subtree covered by a degeneracy class is shown. In the bottom left corner the corresponding elements of the vector $\mathbf{s}$ are listed next to the bonds. To the right, all six different sequences belonging to such degeneracy class are shown together with their codes in terms of the bonds. We write the number of the bond in the code only when it is traversed in the outward (up) direction. It is important to note that the sequences in the same row have the same structure around the vertex 2 while the sequences in the same column share the structure around the vertex 1. One can say that a sequence is made out of building blocks, each representing the structure in the vicinity of a vertex.

This idea is illustrated by Fig. 4.4. In the rounded boxes the possible blocks, or realisations of the local structure of the degeneracy class, are listed.

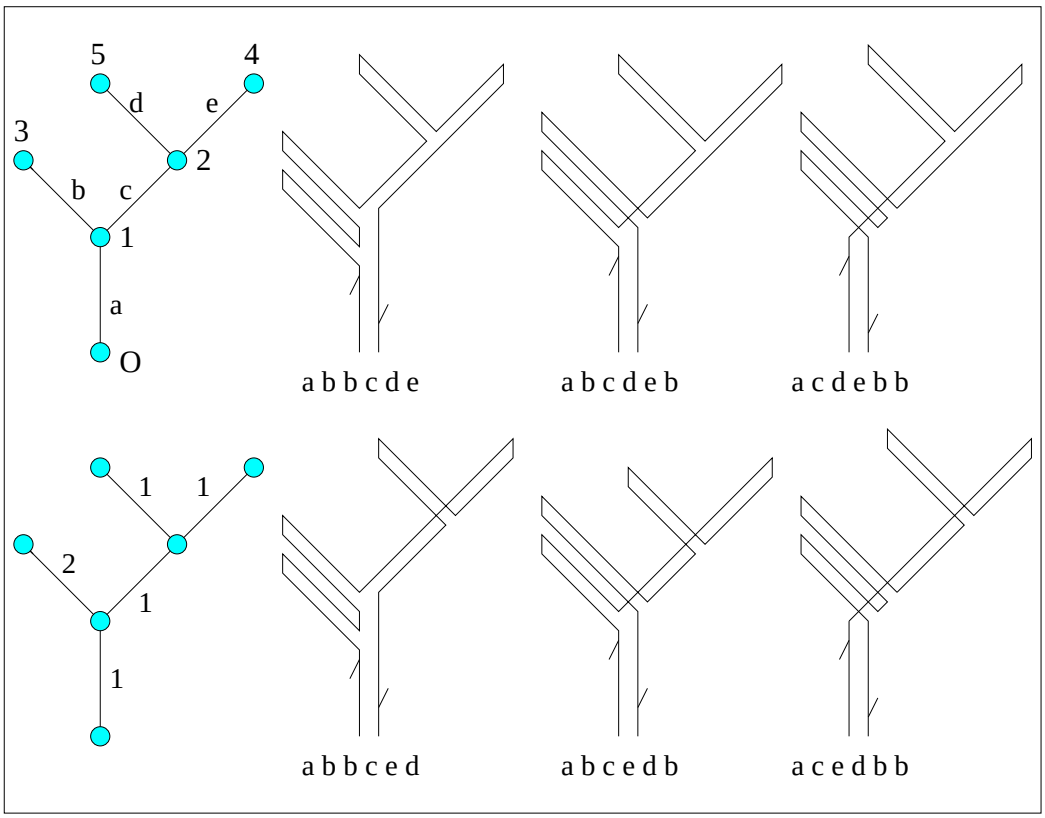

Figure 4.3: An example of degeneracy class. In the top left corner the subtree covered by the degeneracy class is relabelled for convenience. In the bottom left corner the nonzero elements of the vector $\mathbf{s}$ are written next to their bonds. To illustrate the notation introduced in the text, the numbers m_i for the vertex 1 are $m_1 = 1$, $m_2 = 2$ and $m_3 = 1$. To the right, all sequences from the degeneracy class are listed together with their symbolic codes.

To the right from the boxes their local contributions towards $A_{\mathbf{p}}$ are added up. It is not hard to see that if we multiply these sums together we obtain the contribution of the whole degeneracy class, in this case

$$\left(2t_1^3 r_1 + t_1^4\right) \times r_3^2 \times 2t_2^3 \times r_4 \times r_5 = 4r_3^2 t_1^3 r_1 t_2^3 r_4 r_5 + 2r_3^2 t_1^4 t_2^3 r_4 r_5 \qquad (4.2.2)$$

The reason for this factorization is that the behaviour of the sequence on the vertex 2, for example, and the behaviour of the sequence on the vertex 1 are completely independent. The only information that the vertex 1 has about the vertex 2 is that the sequence leaves 1 in the direction of 2 and then comes back. Similarly, all that 1 knows about 3 is the number of times the sequence must leave 1 in the direction 3. This would not be the case if a sequence

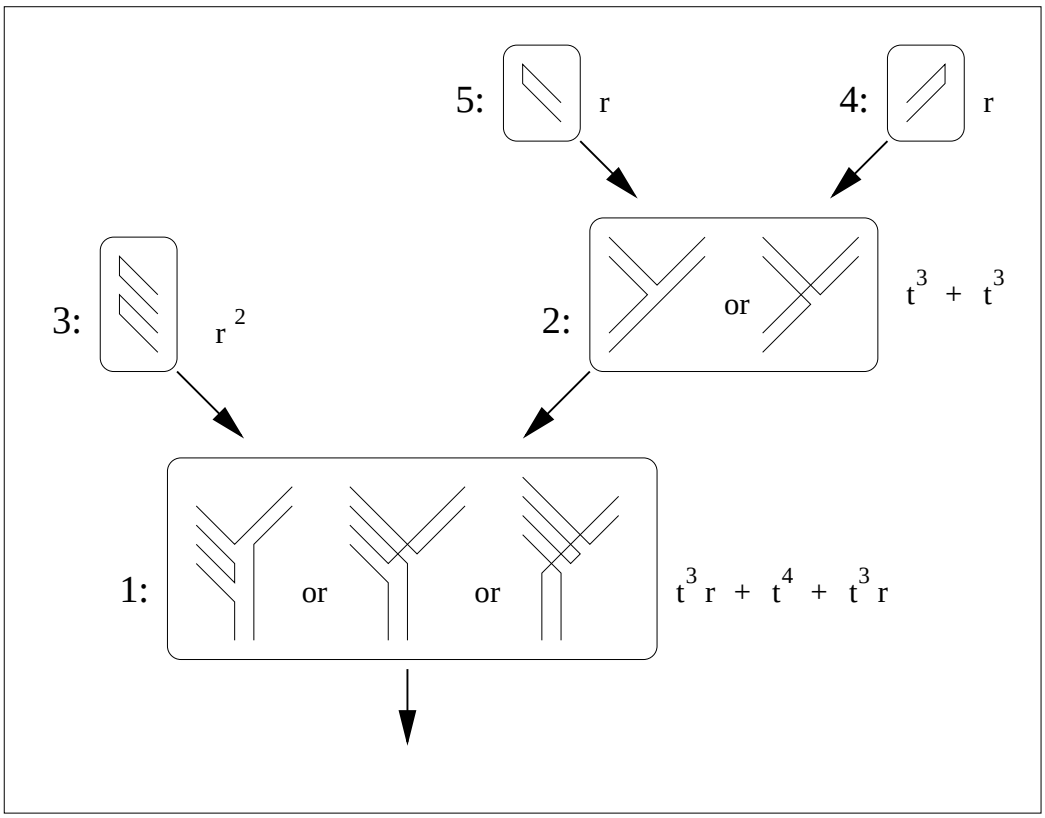

Figure 4.4: Constructing the sequences which belong to the degeneracy class of Fig. (4.3). We make up the sequences using various blocks corresponding to the vertices of the subgraph. The blocks chosen at each vertex are independent: we can use any of the 3 blocks at the vertex 1 together with any of the 2 blocks at the vertex 2. Next to the boxes with the blocks their local contributions are listed. The contribution of the degeneracy class is given by the product of the local ones.

could leave the vertex 1 along the bond b and then come back along the bond c. Fortunately there are no cycles on trees and therefore the factorisation of Eq. (4.2.1) holds.

Now we define another quantity. We will denote

$$U_M(m_1) \equiv \sum_{\mathbf{s}:\, m_1(1)=m_1} \left(\sum_{s(\mathbf{p})=\mathbf{s}} A_{\mathbf{p}} \right)^2 , \tag{4.2.3}$$

the return probability given that the sequence traverses the first bond m_1 times (or *conditional* return probability). Obviously the full probability $P_B(2M)$ is

equal to the sum of $U_M(m_1)$ over m_1,

$$P_B(2M) = \sum_{m_1=1}^{M} U_M(m_1). \tag{4.2.4}$$

It is possible to derive a recursion [21] for the conditional probability $U_M(m_1)$. We restrict ourselves to the case $B = 3$, the generalisation to $B > 3$ will be obvious. We define the upper subtree of the tree G, G_u to be the tree based on the vertices 1, 2, 4, 5, 8, 9, 10, 11 etc, see Fig. 4.1. The lower subtree G_l contains, correspondingly, the vertices 1, 3, 6, 7 etc. The first bond, leading from O to 1 does not belong to either of the subtrees. We are going to use the fact that the subtrees are isomorphic to the original trees.

Given a degeneracy class vector $\mathbf{s}$, we denote by $\mathbf{s}_u$ ($\mathbf{s}_l$) the part of $\mathbf{s}$ which corresponds to the bonds from the upper (correspondingly lower) subtree. Then $\mathbf{s}$ can be expressed as the direct sum $\mathbf{s} = m_1 \oplus \mathbf{s}_l \oplus \mathbf{s}_u$, where m_1 is the number of traversals of the first bond (the bond leading from O to 1). Let us fix the parameters $m_1(1) = m_1$, $m_2(1) = m_2$, $m_3(1) = m_3$, $|\mathbf{s}_u| = M_2 \geq m_2$ and $|\mathbf{s}_l| = M_3 \geq m_3$ such that $m_1 + M_2 + M_3 = M$. Then the contribution of all degeneracy classes with these parameters fixed can be written as

$$\begin{aligned} \sum_{\mathbf{s}} \prod_{v\in\mathcal{V}(G)} \mathcal{U}_v^2 &= \left|\mathcal{U}_1(m_1,m_2,m_3)\right|^2 \left(\sum_{\mathbf{s}_u} \prod_{v\in\mathcal{V}(G_u)} \mathcal{U}_v^2\right)\left(\sum_{\mathbf{s}_l} \prod_{v\in\mathcal{V}(G_l)} \mathcal{U}_v^2\right) \\ &= \left|\mathcal{U}_1(m_1,m_2,m_3)\right|^2 U_{M_2}(m_2) U_{M_3}(m_3), \end{aligned} \tag{4.2.5}$$

where with $\mathcal{U}_v^2$ we abbreviate the squared local contribution of the degeneracy class at the vertex v, $\left|\mathcal{U}_v\left(m_1(v),m_2(v),m_3(v)\right)\right|^2$. Here we used the fact that $\sum_{\mathbf{s}_u}\prod_{v\in\mathcal{V}(G_u)}\mathcal{U}_v^2$ is exactly the conditional return probability on the upper subtree and, since it is isomorphic to the whole tree, their return probabilities are equal. Now we can sum this contribution over all possible choices of previously fixed parameters m_2, m_3, M_2 and M_3 to obtain $U_M(m_1)$:

$$U_M(m_1) = \sum_{M_2+M_3=M-m_1} \sum_{m_2=1}^{M_2} \sum_{m_3=1}^{M_3} \left|\mathcal{U}\left(m_1,m_2,m_3\right)\right|^2 U_{M_2}\left(m_2\right) U_{M_3}\left(m_3\right), \tag{4.2.6}$$

or, for general B,

$$U_M(m_1) = \sum_{M_2+\ldots+M_B=M-m_1} \sum_{m_2=1}^{M_2} \cdots \sum_{m_B=1}^{M_B} \left|\mathcal{U}\left(m_1, m_2, \ldots, m_B\right)\right|^2 \prod_{i=2}^{B} U_{M_i}\left(m_i\right). \tag{4.2.7}$$

Here the summations over M_i are starting from 0 and the summations for m_i are starting from 1 unless the corresponding M_i is equal to 0. If for some i we have $M_i = 0$, the summation over m_i is dropped and the factor $U_{M_i}(m_i)$ is taken to be 1.

4.3 Local contribution of the degeneracy class

In the previous Section we have shown that to determine the return probability we need to calculate the local contribution of degeneracy classes. The local configuration of the tree is the B-star graph and the local information about the degeneracy class is the number of traversals of the bonds of this star. It is clear that calculating the local contribution should be similar to deriving the contribution of the degeneracy classes for star graphs, the feat which was accomplished in Section 3.1.4.

The local numbering of the bonds is arbitrary with the exception of the first bond which points to the origin. We are given B numbers m_i and the question is to find all possible local sequences of bonds where ith bond occurs m_i times. Each sequence is given a weight which is determined according to the usual rules: the weight of the sequence is the product of the weights of the individual transitions with the reflection collecting the factor r and transmission collecting the factor t; the transition between the last bond and the first should also be taken into account. The local contribution is then the sum of these weights over all possible sequences.

Each sequence is characterised by the number of groups of different symbols. If we denote the number of groups of the bond with the local number i by g_i then the weight of the sequence characterised by $m_1, \ldots, m_B$ and $g_1, \ldots, g_B$

is given by $t^G r^{M(v)-G}$, where we introduced the notation $G = g_1 + \ldots + g_b$ and $M(v) = m_1 + \ldots + m_B$. Thus the main question here is how many sequences with the above characteristics are there. To count such sequences we try to relate the number of sequences to the number of sequences $N^{g_1,\ldots,g_j}_{s_1,\ldots,s_j}$, derived in Section 3.1.4.

First of all, while an orbit is a cycle, without a beginning or an end, the sequence is a linear object, with both a beginning and an end. We are interested in all sequences which start with a 1, but we do not demand that it does not end with a 1 (compare to condition (c), Section 3.1.4). Further, if a sequence ends with a group of 1s, we count the last and the first group of 1 as one group. Thus each orbit corresponds to m_1 sequences: we can cut an orbit before each occurrence of 1, obtaining with each such cut a new sequence. For example, the orbit $(1, 1, 2, 1, 3)$ corresponds to 3 sequences starting with a 1: $[1, 1, 2, 1, 3]$, $[1, 2, 1, 3, 1]$ and $[1, 3, 1, 1, 2]$. If, however, the orbit was a repetition of another orbit, with the repetition number $r_{\mathbf{p}}$, we obtain each sequence $r_{\mathbf{p}}$ times. But then such an orbit was counted as $1/r_{\mathbf{p}}$ in the total number of orbits $N^{g_1,\ldots,g_j}_{m_1,\ldots,m_j}$ thus multiplying by m_1 works with the repetitions too. Therefore the number of all possible sequences characterised by $m_1, \ldots, m_B$ and $g_1, \ldots, g_B$ is given by $m_1 N^{g_1,\ldots,g_j}_{m_1,\ldots,m_j}$,

$$m_1 N^{g_1,\ldots,g_j}_{m_1,\ldots,m_j} = m_1(-1)^G \sum_{k_1,\ldots,k_v} \frac{(-1)^K}{K} \binom{K}{k_1,\ldots,k_v} \prod_{i=1}^{B} \binom{m_i - 1}{g_i - 1} \binom{g_i - 1}{k_i - 1}, \tag{4.3.1}$$

where $K = k_1 + \ldots + k_B$ and $G = g_1 + \ldots + g_B$.. Now if we sum the above expression over all possible choices of g_i, multiplying them by $t^G r^{M(v)-G}$, the

result is the local contribution of a degeneracy class,

$$\begin{aligned}
&\mathcal{U}(m_1, m_2, \ldots, m_B) \\
&= m_1 \sum_{g_1,\cdots,g_B} (-t)^G r^{M(v)-G} \sum_{k_1,\ldots,k_B} \frac{(-1)^K}{K} \binom{K}{k_1, \ldots, k_B} \prod_{i=1}^{B} \binom{m_i - 1}{g_i - 1} \binom{g_i - 1}{k_i - 1} \\
&= m_1 \sum_{k_i=1}^{m_i} \frac{(-1)^K}{K} \binom{K}{k_1, \ldots, k_B} \prod_{i=1}^{B} \binom{m_i - 1}{k_i - 1} \sum_{g_i=k_i}^{m_i} \left(\frac{-t}{r}\right)^{g_i} r^{m_i} \binom{m_i - k_i}{g_i - k_i},
\end{aligned} \tag{4.3.2}$$

where the first sum is in fact a B-tuple sum over all k_i. Here we have used the identity

$$\binom{m-1}{g-1}\binom{g-1}{k-1} = \binom{m-1}{k-1}\binom{m-k}{g-k}. \tag{4.3.3}$$

Now, performing the innermost summation

$$\begin{aligned}
\sum_{g_i=k_i}^{m_i} \left(\frac{-t}{r}\right)^{g_i} r^{m_i} \binom{m_i - k_i}{g_i - k_i} &= r^{m_i} \left(\frac{-t}{r}\right)^{k_i} \left(1 - \frac{t}{r}\right)^{m_i} \\
&= (r-t)^{m_i} \left(\frac{-t}{r-t}\right)^{k_i},
\end{aligned} \tag{4.3.4}$$

we finally obtain

$$\begin{aligned}
&\mathcal{U}(m_1, m_2, \ldots, m_B) \\
&\quad = m_1 (r-t)^{M(v)} \sum_{k_i=1}^{m_i} \frac{1}{K} \binom{K}{k_1, \ldots, k_B} \left(\frac{t}{r-t}\right)^K \prod_{i=1}^{B} \binom{m_i - 1}{k_i - 1}.
\end{aligned} \tag{4.3.5}$$

This expression together with the recursion (4.2.7) and Eq. (4.2.4) gives the complete set of exact formulae to determine the return probability.

One can also derive an alternative expression for $\mathcal{U}(m_1, m_2, \ldots, m_B)$. To do so, we represent the factorial $(K-1)!$ as an integral,

$$(K-1)! = \int_0^\infty z^{K-1} \exp(-z) dz \tag{4.3.6}$$

and notice that the summations over different indices k_i become uncoupled. It

leads to the expression

$$\begin{aligned}\mathcal{U}(m_1, m_2, \dots, m_B) &= m_1 (r-t)^{M(v)} \int_0^\infty \exp(-z) \prod_{i=1}^{B} \sum_{k_i=1}^{m_i} \frac{1}{k_i!} \left(\frac{tz}{r-t}\right)^{k_i} \binom{m_i - 1}{k_i - 1} \frac{dz}{z} \\ &= m_1 (r-t)^{M(v)} \int_0^\infty \exp(-z) \prod_{i=1}^{B} L_{m_i}^{-1}(-\alpha z) \frac{dz}{z}, \end{aligned} \tag{4.3.7}$$

where $\alpha = t/(r-t)$ and

$$L_m^{-1}(x) = \sum_{k=1}^{m} \frac{(-x)^k}{k!} \binom{m-1}{k-1}, \tag{4.3.8}$$

is the generalised Laguerre polynomial.

4.3.1 The case $B = 2$

When $B = 2$ the tree is reduced to the line and we should recover the formulae from [21]. To do so we use the combinatorial identity

$$\sum_{j=0}^{m} (-1)^j \binom{a+j}{b} \binom{m}{j} = (-1)^m \binom{a}{b-m} \tag{4.3.9}$$

to simplify the summation

$$(-1)^G \sum_{k_1, \dots, k_B} \frac{(-1)^K}{K} \binom{K}{k_1, \dots, k_B} \prod_{i=1}^{B} \binom{g_i - 1}{k_i - 1} \tag{4.3.10}$$

in the second line of Eq. (4.3.2) in the case $B = 2$. For this summation, denoted R_{g_1, g_2} (see Appendix A.3), one has

$$\begin{aligned} R_{g_1,g_2} &= (-1)^G \sum_{k_2=1}^{g_2} \sum_{k_1=1}^{g_1} \frac{(-1)^{k_1+k_2}}{k_1+k_2} \binom{k_1+k_2}{k_2} \binom{g_1-1}{k_1-1} \binom{g_2-1}{k_2-1} \\ &= (-1)^G \sum_{k_2=1}^{g_2} \frac{(-1)^{k_2+1}}{k_2} \binom{g_2-1}{k_2-1} \sum_{k_1=1}^{g_1} (-1)^{k_1-1} \binom{k_2+k_1-1}{k_2-1} \binom{g_1-1}{k_1-1} \\ &= (-1)^{g_2} \sum_{k_2=1}^{g_2} \frac{(-1)^{k_2}}{k_2} \binom{g_2-1}{k_2-1} \binom{k_2}{k_2-g_1}, \end{aligned} \tag{4.3.11}$$

where we applied identity (4.3.9) with the parameters $j = k_1 - 1$, $a = k_2$, $b = k_2 - 1$, $m = g_1 - 1$. Now using that

$$\frac{1}{k_2}\binom{k_2}{k_2 - g_1} = \frac{1}{g_1}\binom{k_2 - 1}{g_1 - 1} \tag{4.3.12}$$

and applying identity (4.3.9) once again, now with the parameters $j = k_1 - 1$, $a = 0$, $b = g_1 - 1$, $m = g_2 - 1$, we obtain

$$\begin{aligned} R_{g_1,g_2} &= \frac{(-1)^{g_2+1}}{g_1}\sum_{k_2=1}^{g_2}(-1)^{k_2-1}\binom{k_2-1}{g_1-1}\binom{g_2-1}{k_2-1} \\ &= \frac{1}{g_1}(-1)^{g_2+1}(-1)^{g_2-1}\binom{0}{g_1-g_2} = \frac{1}{g_1}\delta_{g_1,g_2}. \end{aligned} \tag{4.3.13}$$

Substituting this result back into the second line of Eq. (4.3.2) we obtain

$$\begin{aligned} \mathcal{U}(m_1,m_2) &= m_1\sum_{g_1,g_2} t^G r^{M(v)-G}\binom{m_1-1}{g_1-1}\binom{m_2-1}{g_2-1}\frac{1}{g_1}\delta_{g_1,g_2} \\ &= \sum_{g_1} t^{2g_1} r^{M(v)-2g_1}\binom{m_1}{g_1}\binom{m_2-1}{g_1-1}, \end{aligned} \tag{4.3.14}$$

which is exactly the corresponding expression from [21].

4.4 Extending results to the complete tree

A natural question to ask is how one can extend the results obtained above to the case of the complete tree, i.e. a tree where all vertices, including the origin, are of valency B. The initial conditions are the same as before: a wave leaving the origin in one chosen direction, see Fig. 4.5.

It turns out that the return probability of such wave packet on the complete tree is related to the quantity we already described, the one-sided conditional return probability $U_M(m)$. Indeed, due to our initial condition, the first bond (the bond $(O, 11)$) is traversed at least once. We denote the number of traversals of this bond by m_1. Now we can introduce an auxiliary vertex β, of valency 2, in the middle of the first bond. We set the amplitudes $t = 1$ and $r = 0$ on this vertex thus the trajectory will never be reflected at the vertex β.

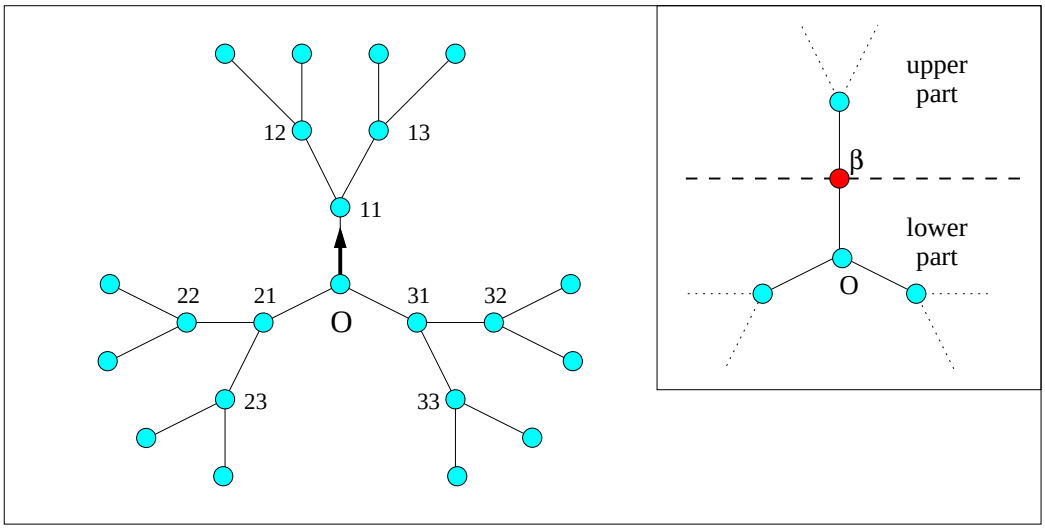

Figure 4.5: Complete infinite tree with $B = 3$. The arrow from the origin indicates the initial wave-packet. Inset: Introducing the auxiliary vertex β which separates the tree into upper and lower parts.

Assume that the sum of all traversals of the bonds in the upper part of the tree, as pictured on Fig. 4.5, is given by M_1, $m_1 \leq M_1 \leq M$. Then the total number of traversals of the bonds in the lower part is $M - M_1 + m_1$, where we add m_1 because the first bond is now split into two. Using the argument similar to the one used to prove Eq. (4.2.5) one can see that the contribution of the sequences characterised by the numbers m_1 and M_1 is given by

$$U_{M_1}(m_1)U_{M-M_1+m_1}(m_1)\mathcal{U}(m_1, m_1), \tag{4.4.1}$$

where $U_{M_1}(m_1)$ is the one-sided conditional return probability to the vertex β from the upper part, $U_{M-M_1+m_1}(m_1)$ is return probability from the lower part and $\mathcal{U}(m_1, m_1)$ is the local contribution at the vertex β. It is easy to see that with our choice of the scattering matrix at β, the local contribution is $\mathcal{U}(m_1, m_1) = 1$. Performing the summation of Eq. (4.4.1) over all possible choices of m_1 and M_1 we obtain the expression for the return probability for the complete tree,

$$P_B^c(2M) = \sum_{m_1=1}^{M} \sum_{M_1=m_1}^{M} U_{M_1}(m_1)U_{M-M_1+m_1}(m_1). \tag{4.4.2}$$

It is interesting to note that the form of the expression is independent of the parameter B.

4.5 Numerical evaluation

4.5.1 Parameters t and r

Before we present the results of the numerical evaluation of Eqs. (4.2.7) and (4.3.5), we discuss the possible values of the amplitudes t and r. These probabilities are the elements of the matrix (4.1.1) which is required to be unitary. Without loss of generality we can assume that r is real: otherwise we can multiply the whole matrix by $\bar{r}/|r|$. If we write t as $t = -|t|e^{i\phi}$, the unitarity condition implies

$$r^2 + (B-1)|t|^2 = 1, \tag{4.5.1}$$

$$2r\cos\phi - (B-2)|t| = 0, \tag{4.5.2}$$

where $\phi \in [0, \pi/2]$ which leads to

$$r = -\left(1 + \frac{4(B-1)}{(2-B)^2}\cos^2\phi\right)^{-1/2} \qquad t = \frac{2r\cos\phi}{2-B}\exp(i\phi). \tag{4.5.3}$$

Note that the reflection amplitude r varies from $(B-2)/B$ (for $\phi = 0$) to 1 ($\phi = \pi/2$) thus the range of possible values of r shrinks as B tends to infinity.

One can consider the matrix $\mathbf{S}^{(v)}$ of a more general form, in fact any unitary matrix would generate consistent dynamics on the tree and thus the diagonal (off-diagonal) elements do not have to be equal. However, taking the elements to be different significantly complicates the expression in Eq. (4.3.5) for $B = 3$ and makes the derivation of such an expression using the same methods impossible for $B > 3$.

An alternative description of r and t can be given in terms of $q = |t|/|r|$, a parameter which has more physical meaning to it than the phase ϕ. If we

assume that t is real then

$$t = \frac{q}{1+q^2(B-1)} \tag{4.5.4}$$

$$r = \frac{-(B-2)q \pm \sqrt{(B-2)^2q^2-4}}{2+2q^2(B-1)}, \tag{4.5.5}$$

where q varies from 0 to $2/(B-2)$ and the connection between ϕ and q is $q = 2\cos(\phi)/(B-2)$.

4.5.2 Computing $\mathcal{U}(m_1, m_2, \ldots, m_B)$

The aim of this Subsection is to simplify the computation of the local contribution $\mathcal{U}(m_1, m_2, \ldots, m_B)$. As given by Eq. (4.3.5), it is a B-fold summation which requires a lot of machine time to evaluate for large m_i. Instead we are going to derive a recursion relation satisfied by $\mathcal{U}$.

First of all we notice that $|r-t|^2 = 1$, which can be easily verified by adding together Eqs. (4.5.1) and (4.5.2). Therefore the factor $(r-t)^m$ in front of the expression for $\mathcal{U}(m_1, m_2, \ldots, m_B)$ can be dropped.

Next we introduce the quantity

$$V_{m_1,m_2,\ldots,m_B} = \mathcal{U}(m_1, m_2, \ldots, m_B)/m_1 \tag{4.5.6}$$

which is symmetric with respect to its argument m_i. We have

$$V_{m_1,m_2,m_3} = \int_0^\infty \exp(-z) L_{m_1}(-\alpha z) L_{m_2}(-\alpha z) L_{m_3}(-\alpha z) \frac{dz}{z}, \tag{4.5.7}$$

where we took $B = 3$ as this case will be of the most interest to us. We also omit the superscript -1 over L. It is well-known [39] that the Laguerre polynomials satisfy the recursion relation (the superscript -1 is omitted!)

$$L_{n+1}(x) = \frac{2n-x}{n+1} L_n(x) - \frac{n-1}{n+1} L_{n-1}(x), \tag{4.5.8}$$

which can be easily proved using the techniques described in [40]. However, if we put the recursion (4.5.8) straight into Eq. (4.5.7) it will do us no good because of the non-numerical factor x multiplying $L_n(x)$. Instead we reformulate

the above recursion in the form

$$xL_n(x) = -(n+1)L_{n+1}(x) + 2nL_n(x) - (n-1)L_{n-1}(x), \tag{4.5.9}$$

and apply it twice to the product $L_{m_1+1}(x)L_{m_2}(x)$, first as (4.5.8) with $n = m_1$ and then as (4.5.9) with $n = m_2$,

$$\begin{aligned}(m_1+1)&L_{m_1+1}(x)L_{m_2}(x) \\ &= 2m_1 L_{m_1}(x)L_{m_2}(x) - xL_{m_1}(x)L_{m_2}(x) - (m_1-1)L_{m_1-1}(x)L_{m_2}(x) \\ &= 2m_1 L_{m_1}(x)L_{m_2}(x) + (m_2+1)L_{m_1}(x)L_{m_2+1}(x) - 2m_2 L_{m_1}(x)L_{m_2}(x) \\ &\quad + (m_2-1)L_{m_1}(x)L_{m_2-1}(x) - (m_1-1)L_{m_1-1}(x)L_{m_2}(x). \end{aligned} \tag{4.5.10}$$

Substituting the above recursion in the integral definition of V_{m_1,m_2,m_3} we find that it satisfies a similar relation,

$$\begin{aligned}(m_1+1)V_{m_1+1,m_2,m_3} &= (m_2+1)V_{m_1,m_2+1,m_3} + 2(m_1-m_2)V_{m_1,m_2,m_3} \\ &\quad + (m_2-1)V_{m_1,m_2-1,m_3} - (m_1-1)V_{m_1-1,m_2,m_3}. \end{aligned} \tag{4.5.11}$$

4.5.3 Results of the simulations

In our simulations we computed the conditional return probability $U_M(m)$ for the branching number $B = 3$ and then performed the summation either according to Eq. (4.2.4) to get the return probability $P_3(2M)$, or according to Eq. (4.4.2) to obtain the return probability for the complete tree, $P_3^c(2M)$. We assumed the matrices $\mathbf{S}^{(v)}$ to be the same for all vertices v, apart form O, which is clearly special. Thus the probabilities t and r were taken to be the same throughout the tree.

First of all we would like to compare the quantum return probability to its classical analogue. We turn our tree into the probabilistic system with the rules similar to the quantum ones. The state is specified by the bond and the direction; the reflection (i.e. change of the direction) has probability $|r|^2$ and the transmission to one of the 2 adjacent bonds happens with probability $|t|^2$.

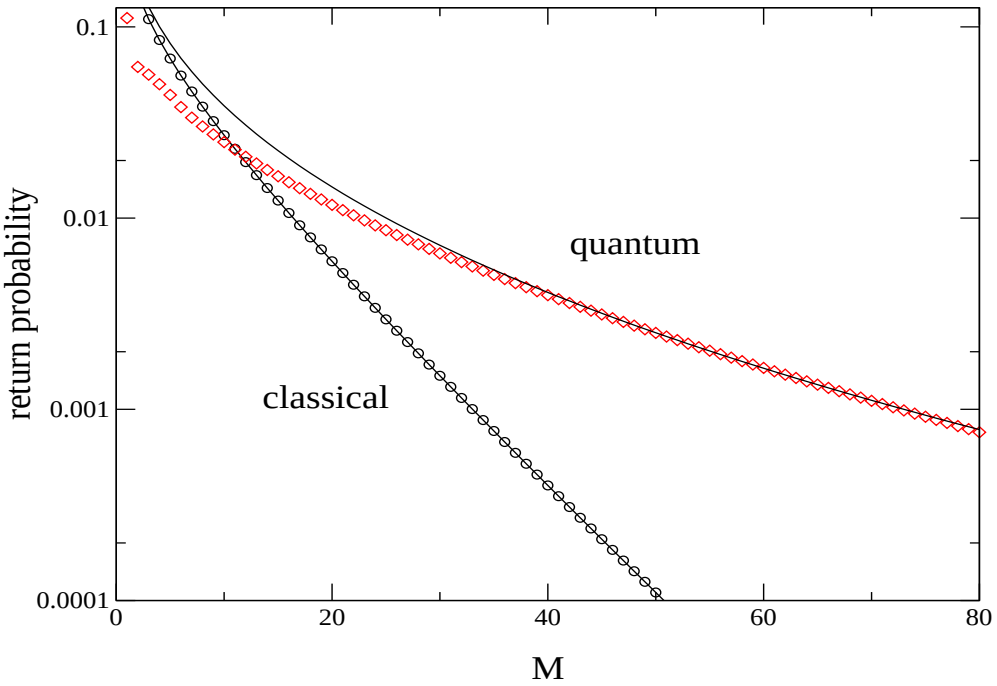

Figure 4.6: Linear-log plot of the quantum (diamonds) and classical (circles) return probabilities for the complete trees with the branching $B = 3$. Here we take the value of $\phi = \pi/3$ which corresponds to $|t|^2 = |r|^2 = 1/3$. The line fitted to the quantum return probability is given by $\exp\{-1.36M^{0.39}\}$.

Since the classical return probability is not really crucial to our exposition, we will only give an upper bound for it in the case when $|r|^2 = |t|^2 = 1/3$ and the tree is complete,

$$P_{cl}(2M) \leq \left(\frac{2}{9}\right)^M \binom{2M-1}{M} \sim \left(\frac{8}{9}\right)^M \frac{1}{\sqrt{2M\pi}} \qquad \text{as } M \to \infty. \quad (4.5.12)$$

The corresponding quantum case is given by $\phi = \pi/3$ and the result of the comparison is presented on Fig. 4.6. As is clear from the plot, the quantum return probability decays to zero but does it at a slower rate than the corresponding classical quantity.

If we are to look for the localisation, however, the natural candidate would be the region of ϕ close to $\pi/2$. For $\phi = \pi/2$ the answer is trivial: the reflection amplitude r is equal to one and $t = 0$ so that the trajectory is confined to the first bond and therefore $P_B(2M) = 1$ for any integer M. Thus we automatically get localisation. The real question is whether we get the localisation for any value of ϕ other than $\pi/2$. The return probability for several values of ϕ close

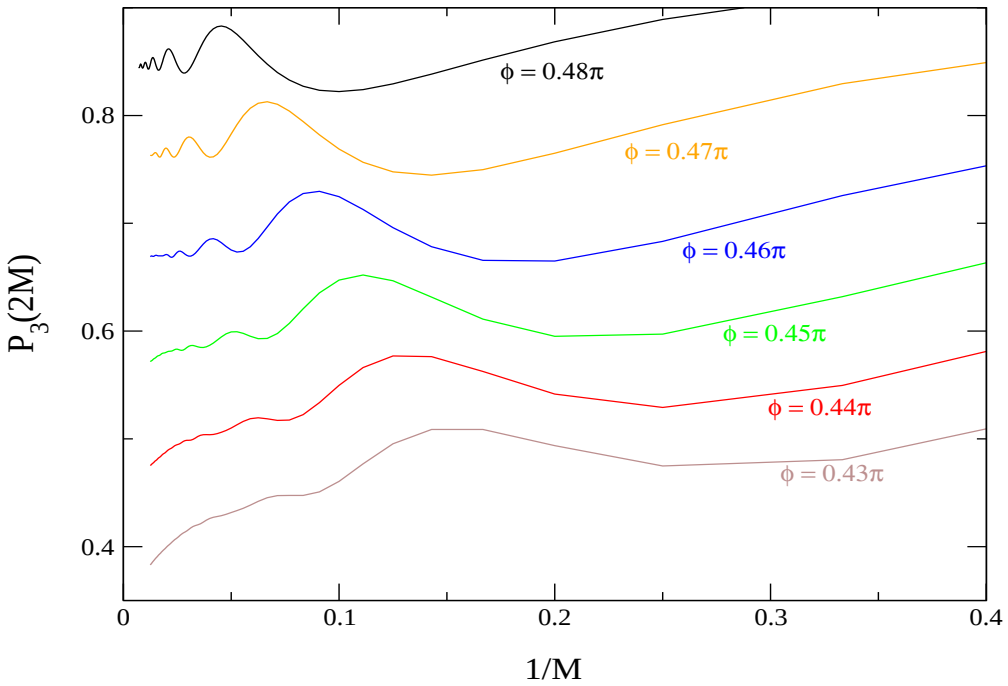

Figure 4.7: Plot of the quantum return probability $P_3(2M)$ for several values of the parameter ϕ, as indicated, versus the inverse number of steps $1/M$. In all cases the value of $P_3(2M)$ was computed up to $M_{\max} = 80$ (except $\phi = 0.48\pi$ where $M_{\max} = 140$). The limiting value of $P_3(2M)$ corresponds to the projected intersection with the y-axis. However the lower three curves are not likely to have a nonzero limiting value as they bend down while approaching the y-axis.

to $\pi/2$ is plotted on Fig. 4.7. It can be seen from the plot that for bigger ϕ the return probability $P_3(2M)$ tends to a nonzero limit as $1/M \to 0$ but for $\phi \leq 0.45\pi$ the plots of $P_3(2M)$ bend down considerably.

An enlarged plot of $P_3(2M)$ for the larger values of ϕ is shown on Fig. 4.8. It seems plausible that all three curves have a nonzero limit. On the contrary, the plots for other 3 values of ϕ seem to decay as M^α which is illustrated by the corresponding fit on Fig. 4.9.

We also tried to fit the curves for $\phi = 0.46\pi$ and $\phi = 0.47\pi$ to a function of the form βM^α. The resulting α is less than zero but it is inevitable for any decreasing function. The exponents α for different values of ϕ are plotted on Fig. 4.10. The drastic change of behaviour of α at $\phi = 0.46\pi$ is remarkable. Basing on this plot we conjecture that the transition between localisation and

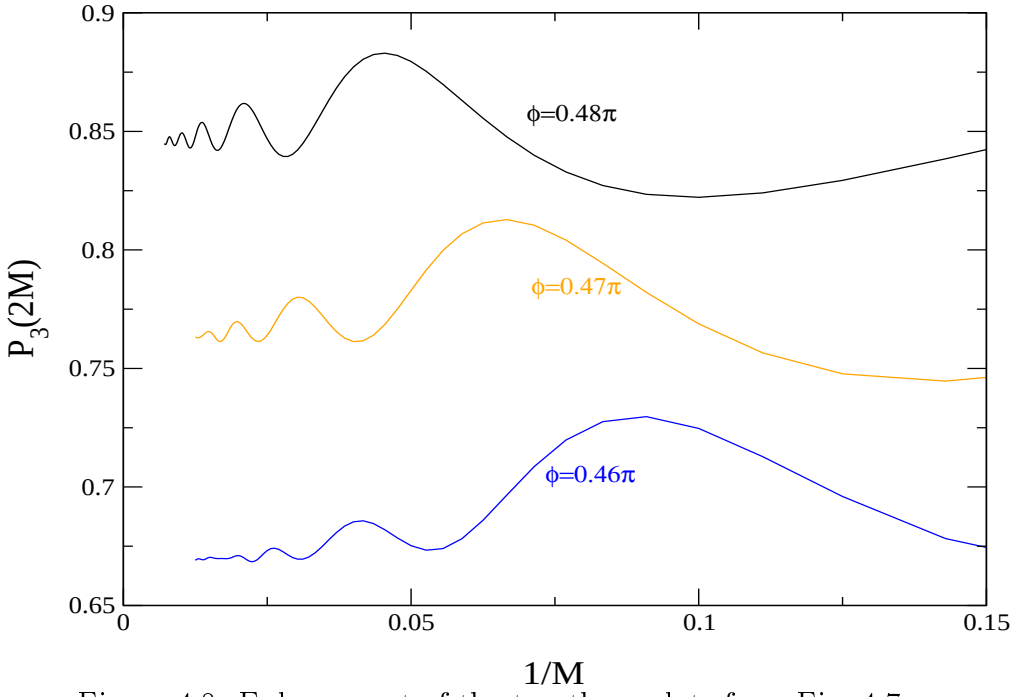

Figure 4.8: Enlargement of the top three plots from Fig. 4.7.

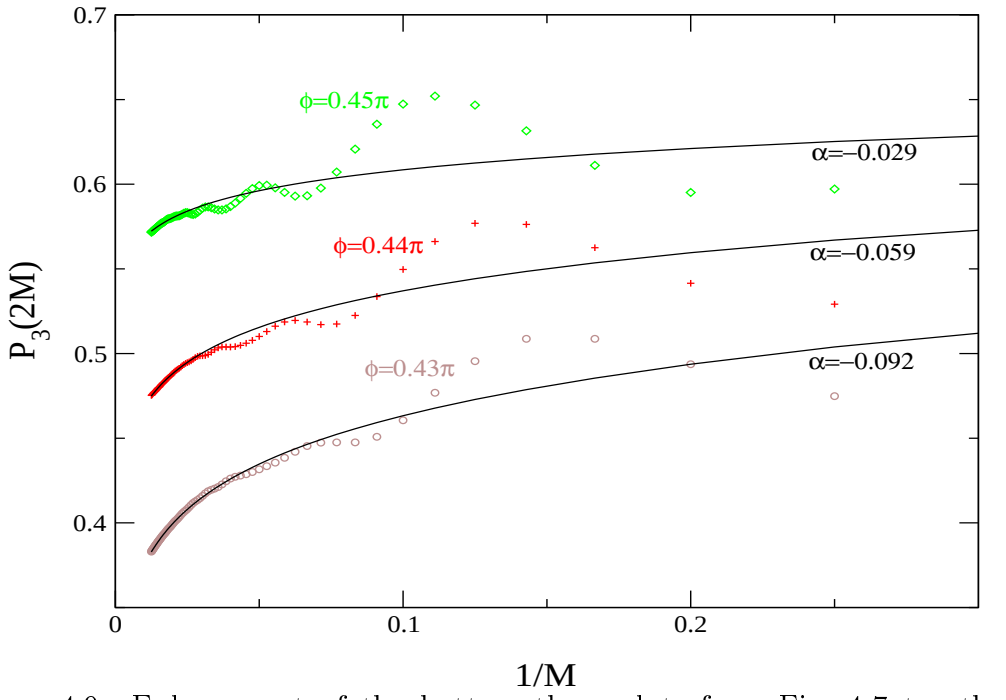

Figure 4.9: Enlargement of the bottom three plots from Fig. 4.7 together with the fitted functions of the form βM^{α}. The corresponding values of the exponent α are indicated on the plot.

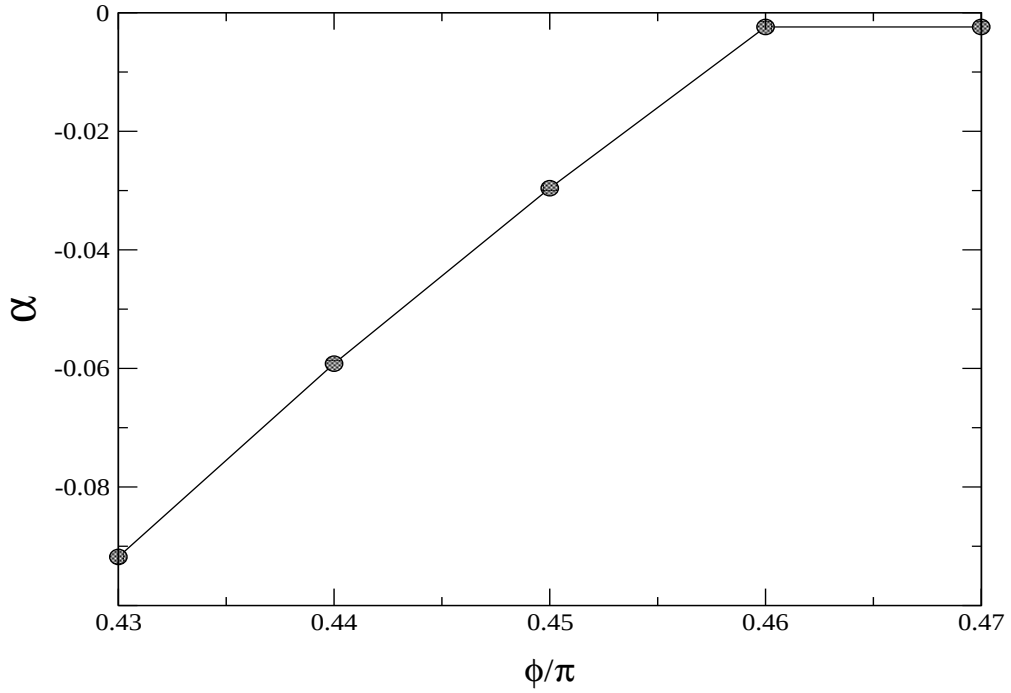

Figure 4.10: The exponent α obtained from by fitting βM^{α} to the tail of $P_3(2M)$ for various ϕ.

delocalisation occurs around $\phi = 0.46\pi$.

Since our model and the model of [31] are not identical, one cannot draw exact analogies between the two. But there is a rough correspondence between ϕ and the parameter θ of [31], it is $2\cos\phi = |t|/|r| = 1/\sinh\theta$. The localisation in [31] was predicted in the range $\theta \in [1.88, \infty)$ which corresponds to $\phi \in [0.45\pi, 0.5\pi]$, showing a good agreement between the two results.

4.6 Large B limit

In this section we show a way to get an expansion of the return probability in the limit $B \to \infty$. The idea of the expansion is similar to what was done in Chapter 3. First, we conjecture that the limit

$$P(\tau) = \lim_{B\to\infty} P_B(B\tau) \tag{4.6.1}$$

exists and is analytic in some neighbourhood of zero. This rescaled return probability $P(\tau)$ is the function we are going to expand.

We set the parameters t and r to be

$$t = 2/B \qquad r = 2/B - 1. \tag{4.6.2}$$

This selection simplifies Eq. (4.3.5) since $r - t = -1$. Besides we do not loose generality with such selection. Indeed, from Eq. (4.5.3) (or Eq. (4.5.4)) it follows that any selection of $|t_B|$ would go to zero at least as B^{-1}. If it decreases faster than B^{-1}, the expansion below would become trivial and therefore non-interesting. Thus we should fix $|t_B| \propto B^{-1}$ which is adequately reflected in Eq. (4.6.2).

This selection makes the sequences with the least number of transitions t more significant in the limit $B \to \infty$. The largest contribution (as in Chapter 3) comes from the sequence which is confined to the first bond[2]. The sequence undergoes $M = B\tau$ rebounds and the corresponding $A_{\mathbf{p}}$ is therefore given by $A_{\mathbf{p}} = (1 - 2/B)^{B\tau}$. Thus the contribution of the sequence to the return probability is

$$K_1(\tau) = \lim_{B\to\infty} (1 - 2/B)^{2B\tau} = \exp(-4\tau). \tag{4.6.3}$$

The next most significant class of sequences consists of the sequences which visit only two bonds because such sequence can have as few as 2 transitions t. Let us consider the contribution made by such sequences in detail.

The first bond in such sequences is fixed while there are $B - 1$ choices for the second bond. We denote the number of traversals (in one chosen direction) of the first bond by m_1 and number of traversals of the second bond by m_2 with the condition $m_1 + m_2 = B\tau$. To calculate A_p we notice that the sequence picks up m_2 rebounds at the end of the second bond and picks up the contribution $\mathcal{U}(m_1, m_2)$ at the vertex where first and second bonds meet. Thus the contribution is

$$K_2(\tau) = \lim_{B\to\infty} (B-1) \sum_{m_2=1}^{B\tau-1} \left|\mathcal{U}(B\tau - m_2, m_2)\right|^2 (1 - 2/B)^{2m_2}. \tag{4.6.4}$$

[2]If we took $|t_B|$ to be decreasing faster than B^{-1}, i.e. if $|t_B|B \to 0$ as $B \to \infty$, this contribution would be equal to 1 while all other contributions would be 0

Denoting m_2/B by q, expanding $\mathcal{U}^2\left(B\tau - m_2, m_2\right)$ according to Eq. (4.3.5), taking the limit $B \to \infty$ termwise and approximating the summation by an integral we obtain

$$\begin{aligned} & K_2(\tau) \\ & = \lim_{B\to\infty} B \sum_{m_2=1}^{B\tau-1} \left| \sum_{k_1,k_2} \frac{(K-1)!}{(k_1-1)!k_2!} \left(\frac{-2}{B}\right)^K \binom{m_1}{k_1} \binom{m_2-1}{k_2-1} \right|^2 \left(1-\frac{2}{B}\right)^{2m_2} \\ & = \int_0^\tau \left((-2)^{k_1+k_2} \frac{(\tau-q)^{k_1} q^{k_2-1} (k_1+k_2-1)!}{k_1!k_2!(k_1-1)!(k_2-1)!} \right)^2 \exp(-4q) dq, \end{aligned} \tag{4.6.5}$$

where $m_1 = B\tau - m_2$ and $K = k_1 + k_2$, and we have made the approximations

$$\frac{1}{B^{k_2-1}} \binom{m_2-1}{k_2-1} \to \frac{q^{k_2-1}}{(k_2-1)!} \quad \text{and} \quad \frac{1}{B^{k_1}} \binom{m_1}{k_1} \to \frac{(\tau-q)^{k_1}}{k_1!}. \tag{4.6.6}$$

Next we expand the square and do the integration term by term using the rule

$$\begin{aligned} \int_0^\tau q^a (\tau-q)^b \exp(-4q) dq &= \sum_{l=0}^\infty \frac{(-4)^l}{l!} \int_0^\tau q^{a+l} (\tau-q)^b dq & (4.6.7) \\ &= \sum_{l=0}^\infty \frac{(-4)^l \tau^{a+b+l+1}}{(a+b+l+1)!} \frac{a!(b+l)!}{l!}. & (4.6.8) \end{aligned}$$

We arrive to

$$\begin{aligned} K_2(\tau) \approx & -\sum_{l=0}^\infty \sum_{k_i=1}^\infty \sum_{n_i=1}^\infty 2^{N+K+2l} \frac{(-\tau)^{K+N+l-1} (k_1+n_1)!(k_2+n_2+l-2)!}{(K+N+l-1)!l!} \\ & \times (K-1)!(N-1)! \prod_{j=1}^2 \frac{1}{k_j! n_j! (k_j-1)!(n_j-1)!}, \end{aligned} \tag{4.6.9}$$

where $K = k_1 + k_2$ and $N = n_1 + n_2$. Since the minimum values for K and N are 2, the expansion of $K_2(\tau)$ starts with τ^3.

The expression for $K_2(\tau)$ is already very complicated, involving summations over five indices. To give a further example, the contribution from the sequence sketched on the inset of Fig. 4.11 can be expressed in the form

$$\begin{aligned} K_{33}(\tau) \approx & \lim_{B\to\infty} \left[2 \binom{B-1}{2} \binom{B-1}{2} B^4 \right. \\ & \left. \times \int_{q_1+\ldots+q_5=\tau} \frac{V^2(q_1,q_2,q_3)}{B^4} \frac{V^2(q_3,q_4,q_5)}{B^4} e^{-4(q_2+q_4+q_5)} d\mathbf{q} \right] \\ = & \frac{1}{2} \int_{q_1+\ldots+q_5=\tau} V^2(q_1,q_2,q_3) V^2(q_3,q_4,q_5) e^{-4(q_2+q_4+q_5)} d\mathbf{q}, \end{aligned} \tag{4.6.10}$$

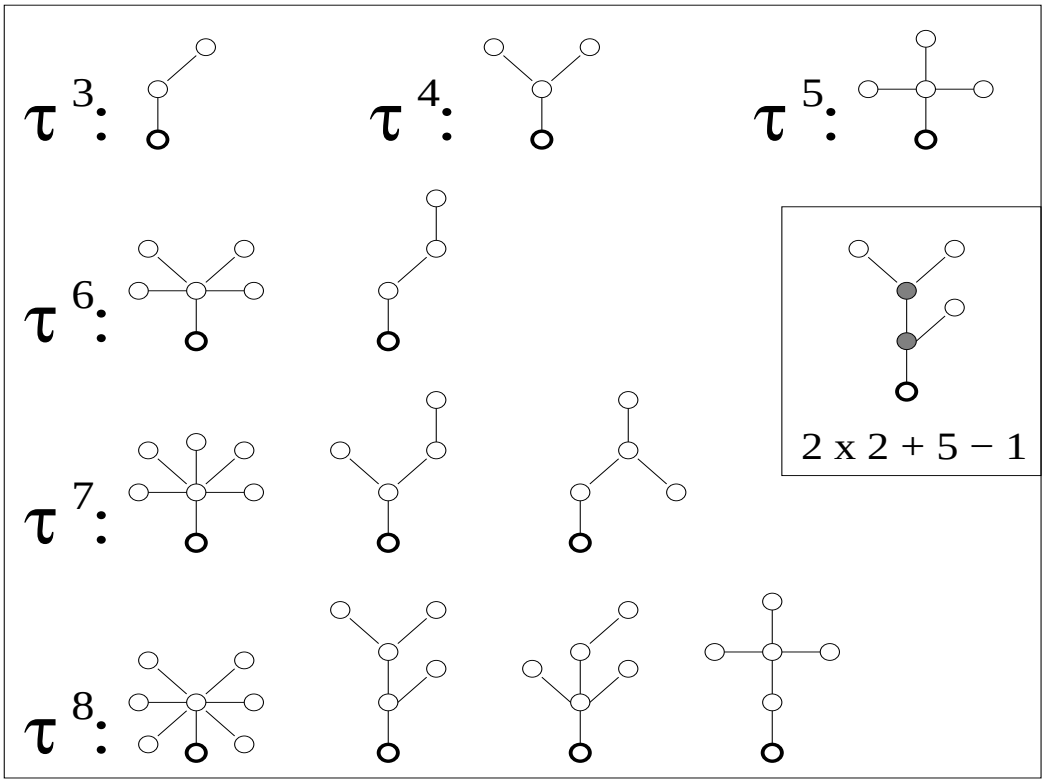

Figure 4.11: The shapes of the periodic sequences whose contribution's expansion starts with the term of order 8 or lower. Thicker circle corresponds to the origin. Inset: calculating the lowest power in the expansion for a sequence. The lowest power is given by twice the number of vertices of valency 2 or greater (shaded circles) plus number of all bonds minus 1.

where $q_i = m_i/B$,

$$\begin{aligned} V(q_1,q_2,q_3) &= \lim_{B\to\infty}\left[B^2\mathcal{U}(Bq_1,Bq_2,Bq_3)\right] \\ &= q_1\sum_{k_1,k_2,k_3\geq 1}\frac{(-2)^K}{K}\binom{K}{k_1,k_2,k_3}\prod_{i=1}^{3}\frac{q_i^{k_i-1}}{(k_i-1)!} \end{aligned} \tag{4.6.11}$$

and the integral is taken over $\sum_{i=1}^{5} q_i = \tau$, i.e. the integration is over four variables q_2, q_3, q_4, and q_5, with $q_1 = \tau - q_2 - q_3 - q_4 - q_5$. Although it is possible to perform the integration to obtain an explicit expression for the coefficients of the τ expansion, the expression is incredibly bulky. It is clear, though, that the expansion starts from the power τ^8.

Fig. 4.11 lists the shapes of periodic sequences whose contribution starts from the term of order 8 or below.

Proposition 5. *For a general shape (subtree), the lowest power in the expansion of the corresponding contribution to $P(\tau)$ is given by twice the number of the vertices in the subtree with valency greater than 1 plus the number of bonds of the subtree minus one.*

Indeed, each vertex of the valency greater than 1 will produce the factor $V^2(q_i, \ldots, q_j)$ whose expansion starts with the term of order q_i^2 (it corresponds to taking the parameters $k_i = \ldots = k_j = 0$ in the sum of Eq. (4.6.11)). Then the integration will add the power equal to the number of the bonds of the subtree minus one — the number of free variables in the integration.

Chapter 5

Integral Representation

In this Chapter we return to the star graphs. But now we will approach the problem of deriving the statistics not through the trace formula and the periodic orbits but by using the secular equation (2.2.12) directly. One can evaluate the determinant and obtain a (transcendental) equation on k for any given graph, but for star graphs it takes an especially simple form,

$$\sum_{j=1}^{B} \tan L_j k = 0. \tag{5.0.1}$$

Our aim is to derive an expression for the two point correlation function in the limit $B \to \infty$ and to compare it with the expansion of the form factor we obtained in Chapter 3. The derivation is based on the method developed in [32] for statistics of the Šeba billiard [33, 34].

5.1 Statement of the problem

Here we consider an alternative approach to the question of calculating the spectral statistics. Instead of averaging over a large spectral interval we apply the averaging with respect to the lengths of the individual bonds. That is we assume that the lengths L_j are independent random variables distributed uniformly on the interval $[L_0, L_0 + \Delta L]$ and redefine the two-point correlation

function as

$$R_2(x) = \lim_{k\to\infty} \frac{1}{\bar{d}^2} \left\langle d(k) d\left(k + \frac{x}{\bar{d}}\right) \right\rangle_{\{L_j\}}, \tag{5.1.1}$$

where $d(x)$, as before, is the spectral density. The averaging is defined by

$$\langle \cdot \rangle_{\{L_j\}} = \int_{L_0}^{L_0+\Delta L} \cdots \int_{L_0}^{L_0+\Delta L} \cdot \quad \frac{dL_1}{\Delta L} \cdots \frac{dL_B}{\Delta L}. \tag{5.1.2}$$

We argue that definition (5.1.1) produces an equivalent result to the one considered in Section 2.6.2. Indeed, imaging applying the averaging to a term of the form $\cos\left((l_{\mathbf{q}} - l_{\mathbf{p}})k + l_{\mathbf{q}}\frac{2\pi x}{L}\right)$, see Eq. (2.6.21). We can write $l_{\mathbf{p}}$ as $s_{1,\mathbf{p}}L_1 + \ldots + s_{B,\mathbf{p}}L_B$, where the vector $\mathbf{s_p}$ is the vector of the bond staying rates of the orbit $\mathbf{p}$. Similarly $l_{\mathbf{q}} = s_{1,\mathbf{q}}L_1 + \ldots + s_{B,\mathbf{q}}L_B$ and if for some j the corresponding staying rates $s_{j,\mathbf{p}}$ and $s_{j,\mathbf{q}}$ are not equal then after averaging with respect to L_j the cosine term will acquire a factor of order $1/k$. Thus all contributions from the pairs of orbits of different length will disappear in the limit $k \to \infty$, recovering Eq. (2.6.22). Unfortunately it is hard to put this argument into a more rigorous form.

In this section we make the following assumptions

- we are interested in the limits $\Delta L \to 0$ and $B \to \infty$.
- when the limits $\Delta L \to 0$ and $k \to \infty$ are to be taken together we assume that $k\Delta L \to \infty$.

In what follows we will not concern ourselves with the periodic orbits. On the contrary, we will derive a formula for $R_2(x)$ from the "first principles".

The general solution of Eq. (2.1.22) on a star graph can be written in the form $\Psi_{0,j}(x) = A_j \cos(k(x + \phi_j))$, $j = 1, \ldots, B$. Applying the current conservation condition, (2.1.21), on the outer vertices ($x = L_j$), we obtain $\phi_j = -L_j$. Condition (2.1.20) on the central vertex implies $A_j \cos(L_j k) =$ const. Finally, applying condition (2.1.21) and dividing by $A_j \cos(L_j k)$ we obtain

$$\sum_{j=1}^{B} \tan L_j k = 0. \tag{5.1.3}$$

Thus k is an eigenlevel if and only if it is a zero of the function

$$F(k) = \sum_{j=1}^{B} \tan L_j k. \tag{5.1.4}$$

Now we remember that for any function $F(k)$ the density

$$d(k) = \sum_n \delta(k - k_n), \tag{5.1.5}$$

of the zeros $\{k_n\}$ of F can be expressed as

$$d(k) = |F'(k)|\delta(F(k)) = \frac{1}{2\pi} \int |F'(k)| e^{izF(k)} dz, \tag{5.1.6}$$

where the integral is taken over the whole real line. In our case $F(k) = \sum_{j=1}^{B} \tan L_j k$ and thus

$$d(k) = \frac{1}{2\pi} \int \sum_{s=1}^{B} \frac{L_s}{\cos^2 L_s k} e^{iz \sum_{j=1}^{B} \tan L_j k} dz. \tag{5.1.7}$$

5.2 Average density

First of all we would like to calculate the average density $\overline{d}$ now defined as

$$\bar{d} = \lim_{\Delta L \to 0, k \to \infty} \Big\langle d(k) \Big\rangle_{\{L_j\}} \tag{5.2.1}$$

and compare it to the result we derived in Subsection 2.6.1. Applying the averaging (5.1.2) to Eq. (5.1.7) we obtain

$$\begin{aligned} \Big\langle d(k) \Big\rangle_{\{L_j\}} &= \frac{1}{2\pi} \int_{-\infty}^{\infty} dz \sum_{s=1}^{B} \int \cdots \int_{L_0}^{L_0+\Delta L} L_s \frac{e^{iz \sum_{j=1}^{B} \tan kL_j}}{\cos^2 kL_s} \frac{dL_1}{\Delta L} \cdots \frac{dL_B}{\Delta L} \\ &= \frac{B}{2\pi} \int_{-\infty}^{\infty} dz \left(\int_{L_0}^{L_0+\Delta L} e^{iz \tan kL} \frac{dL}{\Delta L} \right)^{B-1} \left(\int_{L_0}^{L_0+\Delta L} L \frac{e^{iz \tan kL}}{\cos^2 kL} \frac{dL}{\Delta L} \right) \\ &\equiv \frac{B}{2\pi} \int_{-\infty}^{\infty} \tilde{f}^{B-1}(z) \tilde{g}(z)\, dz. \end{aligned} \tag{5.2.2}$$

Here the function $g(z)$ is

$$\tilde{g}(z) = \int_{L_0}^{L_0+\Delta L} L \frac{e^{iz \tan kL}}{\cos^2 kL} \frac{dL}{\Delta L} \approx \frac{L_0}{\Delta L k} \int_{L_0}^{L_0+\Delta L} e^{iz \tan kL} \frac{\partial \tan kL}{\partial L}\, dL, \tag{5.2.3}$$

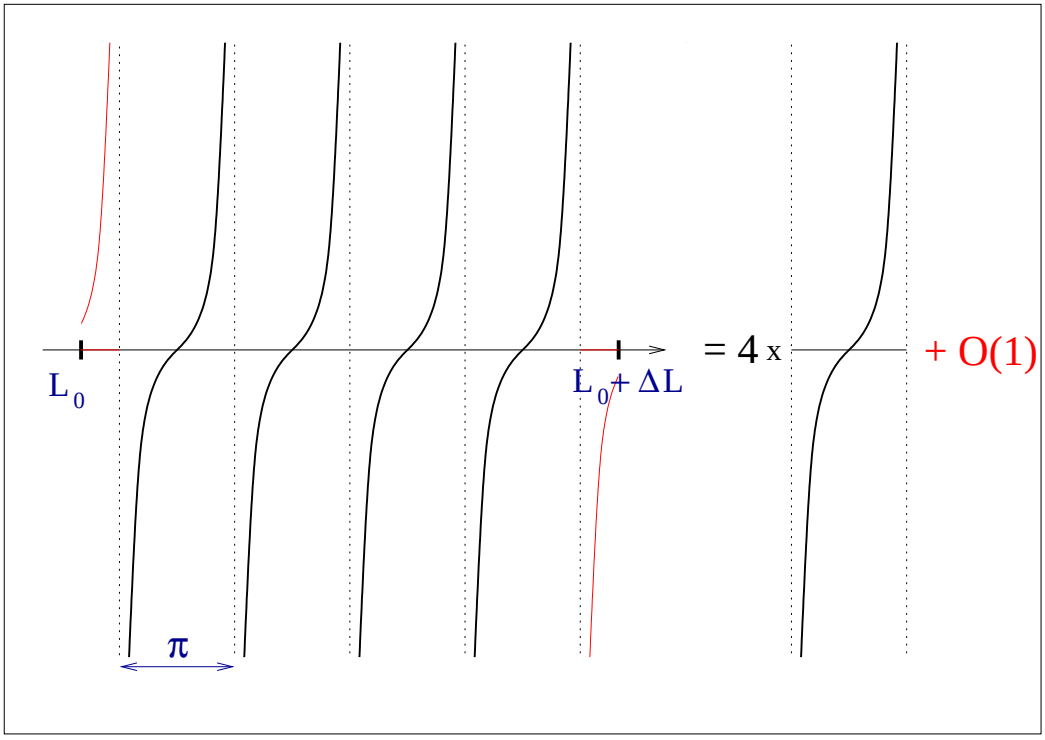

Figure 5.1: Illustration to the transition from Eq.(5.2.3) to Eq. (5.2.4): the interval $[L_0, L_0 + \Delta L]$ contains approximately $k\Delta L/\pi$ periods of $\tan kL$. The incomplete bits of the period on the left and right give the $O(1)$ contribution.

where we were able to approximate L by L_0 because it is slowly varying, comparing to $\tan kL$, and ultimately we will take the limit $\Delta L \to 0$. Now, since $\tan kL$ is a periodic function with the period of π/k and the integration is performed over the interval containing approximately $\Delta Lk/\pi$ periods, see Fig. 5.1, we can further approximate

$$\begin{aligned} \tilde{g}(z) &= \frac{L_0}{\Delta Lk}\left(\frac{\Delta Lk}{\pi}\int_{-\pi/(2k)}^{\pi/(2k)} e^{iz\tan kL}\frac{\partial \tan kL}{\partial L}\, dL + O(1)\right) \qquad (5.2.4)\\ &\approx \frac{L_0}{\pi}\int_{-\infty}^{\infty} e^{iz\alpha} d\alpha = 2L_0\delta(z), \end{aligned}$$

where $O(1)$ is a quantity which is bounded as $\Delta Lk \to \infty$ and $\alpha = \tan kL$. Similarly for the function $\tilde{f}(z)$,

$$\begin{aligned} \tilde{f}(z) &= \int_{L_0}^{L_0+\Delta L} e^{iz\tan kL}\frac{dL}{\Delta L} = \frac{L_0}{\Delta Lk}\int_{L_0}^{L_0+\Delta L} e^{iz\tan kL}\frac{d\tan kL}{1+\tan^2 kL}\\ &\approx \frac{1}{\pi}\int_{-\infty}^{\infty}\frac{e^{iz\alpha}}{1+\alpha^2}d\alpha = e^{-|z|}, \qquad (5.2.5) \end{aligned}$$

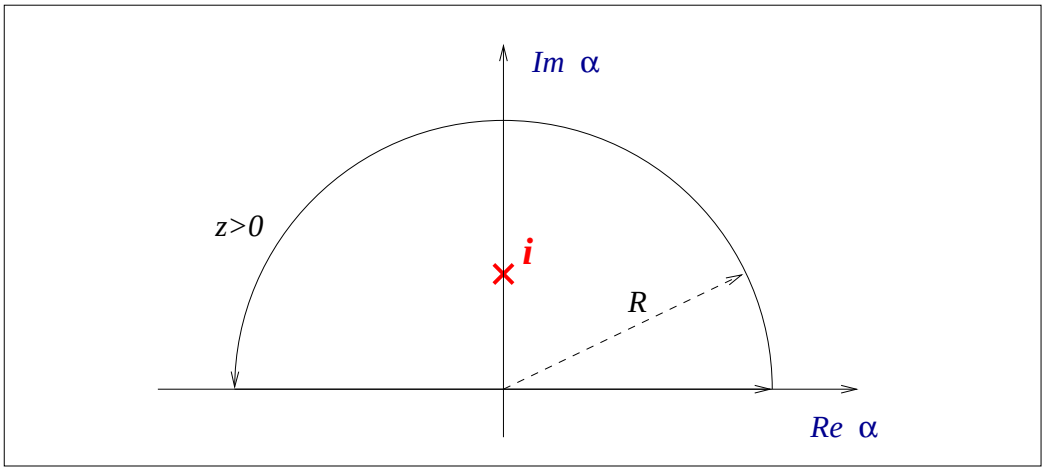

Figure 5.2: Closing the contour in the integral of Eq. (5.2.5) in the case $z > 0$. Along the arc the integral is bounded by $1/R$. The residue at the pole is equal to πe^{iz}.

where the last integral was evaluated by closing the contour in either the upper ($z > 0$, see Fig. 5.2) or lower ($z < 0$) half-plane.

Substituting the results into Eq. (5.2.2) we obtain for the average density

$$\bar{d} = \frac{B}{2\pi} 2L_0 \int_{-\infty}^{\infty} e^{-(B-1)|z|} \delta(z) dz = \frac{L_0 B}{\pi}, \tag{5.2.6}$$

which coincides with the expression of Eq.(2.6.5).

5.3 Two-point correlation function

5.3.1 The recipe

To shorten the notation we introduce the function

$$\begin{aligned} R(k_1, k_2) &= \langle d(k_1) d(k_2) \rangle \qquad (5.3.1) \\ &= \left\langle \int_{-\infty}^{\infty} \sum_{r,s=1}^{B} \frac{L_r L_s e^{i \sum_{j=1}^{B} (z_1 \tan k_1 L_j + z_2 \tan k_2 L_j)}}{\cos^2 k_1 L_r \cos^2 k_2 L_s} \frac{d\mathbf{z}}{4\pi^2} \right\rangle_{\{L_j\}}, \end{aligned}$$

where $\mathbf{z} = (z_1, z_2)$. Then the two-point correlation function is given by

$$R_2(x) = \lim_{k \to \infty} \frac{1}{\bar{d}^2} R\left(k, k + \frac{x}{\bar{d}}\right), \tag{5.3.2}$$

where $\bar{d}$ is the mean density.

Applying the averaging, as was done in Eq. (5.2.2), to the integral in Eq. (5.3.1) we reduce it to

$$R(k_1,k_2)=\int_{-\infty}^{\infty}\left\{Bg(\mathbf{z})f^{B-1}(\mathbf{z})+(B^2-B)\phi_1(\mathbf{z})\phi_2(\mathbf{z})f^{B-2}(\mathbf{z})\right\}\frac{d\mathbf{z}}{4\pi^2}, \quad (5.3.3)$$

where

$$f(\mathbf{z}) = \frac{1}{\Delta L}\int_{L_0}^{L_0+\Delta L} e^{i(z_1\tan(k_1L)+z_2\tan(k_2L))}dL \quad (5.3.4)$$

$$g(\mathbf{z}) = \frac{1}{\Delta L}\int_{L_0}^{L_0+\Delta L} \frac{L^2}{\cos^2 k_1L\cos^2 k_2L}e^{i(z_1\tan(k_1L)+z_2\tan(k_2L))}dL \quad (5.3.5)$$

$$\phi_1(\mathbf{z}) = \frac{1}{\Delta L}\int_{L_0}^{L_0+\Delta L} \frac{L}{\cos^2 k_1L}e^{i(z_1\tan(k_1L)+z_2\tan(k_2L))}dL \quad (5.3.6)$$

$$\phi_2(\mathbf{z}) = \frac{1}{\Delta L}\int_{L_0}^{L_0+\Delta L} \frac{L}{\cos^2 k_2L}e^{i(z_1\tan(k_1L)+z_2\tan(k_2L))}dL. \quad (5.3.7)$$

5.3.2 The ingredients

Substituting $k_1=k$, $k_2=k+\pi x/(BL_0)$ for fixed x and taking the limits $k\to\infty$, $\Delta L\to 0$ (while $k\Delta L\to\infty$) we obtain for the first integral

$$\begin{aligned} f(\mathbf{z}) &= \frac{1}{\Delta L}\int_{L_0}^{L_0+\Delta L} e^{i\left(z_1\tan(kL)+z_2\tan\left(kL+\frac{\pi xL}{BL_0}\right)\right)}dL \\ &\approx \frac{1}{\pi}\int_{-\pi/2}^{\pi/2} e^{i\left(z_1\tan\phi+z_2\tan\left(\phi+\frac{\pi x}{B}\right)\right)}d\phi, \end{aligned} \quad (5.3.8)$$

where we put $L/L_0\approx 1$ because it is slowly varying and, as in transition from Eq. (5.2.3) to Eq. (5.2.4), we approximated f by the integral over one period length. We write

$$\tan\left(\phi+\frac{\pi x}{B}\right)=\frac{\tan\phi+\tan\left(\frac{\pi x}{B}\right)}{1-\tan\phi\tan\left(\frac{\pi x}{B}\right)}=\frac{1+\beta^2}{\beta-\tan\phi}-\beta, \quad (5.3.9)$$

where $\beta=(\tan(\pi x/B))^{-1}\propto B/(\pi x)$ (we are interested in $B\to\infty$ limit). Performing the change of variables $\alpha=\tan\phi-\beta$, we arrive to

$$f(z_1,z_2)\approx\frac{e^{i\beta(z_1-z_2)}}{\pi}\int_{-\infty}^{\infty}e^{iz_1\alpha-iz_2\frac{\beta^2+1}{\alpha}}\frac{d\alpha}{(\alpha+\beta)^2+1}, \quad (5.3.10)$$

Note that $f(\mathbf{z})$ is invariant under exchange $z_1\leftrightarrow z_2$ and $\beta\to-\beta$, which can be verified by the change of variables $\alpha=(\beta^2+1)/y$ in Eq. (5.3.10).

To evaluate the integral of Eq. (5.3.10) we differentiate it with respect to z_1 and z_2 to get

$$\begin{aligned}\frac{\partial f}{\partial z_1}-\frac{\partial f}{\partial z_2} &= i\frac{e^{i\beta(z_1-z_2)}}{\pi}\int_{-\infty}^{\infty} e^{iz_1\alpha-iz_2\frac{\beta^2+1}{\alpha}}\left(2\beta+\alpha+\frac{\beta^2+1}{\alpha}\right)\frac{d\alpha}{(\alpha+\beta)^2+1} \\ &= i\frac{e^{i\beta(z_1-z_2)}}{\pi}\int_{-\infty}^{\infty} e^{iz_1\alpha-iz_2\frac{\beta^2+1}{\alpha}}\frac{d\alpha}{\alpha} = -e^{i\beta(z_1-z_2)}\Phi(z_1,z_2), \quad (5.3.11)\end{aligned}$$

where we denoted

$$\begin{aligned}\Phi(z_1,z_2) &\equiv -\frac{i}{\pi}\int_{-\infty}^{\infty} e^{iz_1\alpha-iz_2\frac{\beta^2+1}{\alpha}}\frac{d\alpha}{\alpha} \quad (5.3.12)\\ &= 2\,\mathrm{sign}(z_1)H(-z_1z_2)J_0\left(2\sqrt{-(\beta^2+1)z_1z_2}\right),\end{aligned}$$

where $J_0(x)$ is the Bessel function of the first kind and $H(x)$ is the Heaviside function (characteristic function of the half axis $[0,\infty)$).

Now to find the function $f(\mathbf{z})$ we need to solve the partial differential equation

$$\frac{\partial f}{\partial z_1}-\frac{\partial f}{\partial z_2} = -e^{i\beta(z_1-z_2)}\Phi(z_1,z_2). \quad (5.3.13)$$

We are going to use the *method of characteristics*, a general method of solving first order PDEs of the form

$$P(\mathbf{z})\frac{\partial f}{\partial z_1}+Q(\mathbf{z})\frac{\partial f}{\partial z_2} = R(\mathbf{z}). \quad (5.3.14)$$

The idea behind the method is to find the foliation of the plane into set of curves $z_1 = z_1(t)$, $z_2 = z_2(t)$ such that the left hand side of the equation is the differential of f with respect to t. It leads to a set of ordinary differential equations, usually written as

$$\frac{dy}{Q(\mathbf{z})} = \frac{dx}{P(\mathbf{z})} = \frac{df}{R(\mathbf{z})}. \quad (5.3.15)$$

In our case $P=1, Q=1$ and $R=-e^{i\beta(z_1-z_2)}\Phi(\mathbf{z})$, and, applying the method, we obtain the solution in the form

$$f(\mathbf{z}) = C(z_1+z_2)+\int_0^{z_1} R\left(y, z_1+z_2-y\right)dy, \quad (5.3.16)$$

where the function $C(\,\cdot\,)$ is to be found from the boundary condition(s). Fixing $z_1 = 0$ we have

$$\begin{aligned} C(z_2) &= f(0,z_2) = f_{\beta\mapsto-\beta}(z_2,0) \\ &= \frac{e^{-i\beta z_2}}{\pi}\int_{-\infty}^{\infty} e^{iz_2\alpha}\frac{d\alpha}{(\alpha-\beta)^2+1} = e^{-|z_2|}, \end{aligned} \tag{5.3.17}$$

which fixes the function $C(\cdot)$. Thus from Eqs. (5.3.11), (5.3.16) and (5.3.17),

$$f(\mathbf{z}) = e^{-|z_1+z_2|} - \int_0^{z_1} e^{i\beta(2y-z_1-z_2)}\Phi\left(y, z_1+z_2-y\right)dy. \tag{5.3.18}$$

We treat the integral for $g(\mathbf{z})$ (see Eq. (5.3.5)) in a fashion similar to the one used to obtain Eq. (5.3.10). This leads us to

$$\begin{aligned} g(z_1,z_2) &\approx \frac{L_0^2}{\pi}\int_{-\pi/2}^{\pi/2}\frac{e^{i(z_1\tan(\phi)+z_2\tan(\phi+\pi x/B))}}{\cos^2(\phi)\cos^2(\phi+\pi x/B)}d\phi \qquad (5.3.19)\\ &= L_0^2\frac{e^{i\beta(z_1-z_2)}}{\pi}\int_{-\infty}^{\infty} e^{iz_1\alpha - iz_2\frac{\beta^2+1}{\alpha}}\left(1+\left(\frac{1+\beta^2}{\alpha}+\beta\right)^2\right)d\alpha, \end{aligned}$$

where we made the change of variable $\alpha = \tan\phi - \beta$ and used the identity

$$\frac{1}{\cos^2(\phi+\pi x/v)} = 1+\tan^2(\phi+\pi x/v) = \left(1+\left(\frac{1+\beta^2}{\tan\phi-\beta}+\beta\right)^2\right). \tag{5.3.20}$$

Comparing the integral above to the definition of the function $\Phi(z_1,z_2)$, Eq. (5.3.12), we note that

$$1+\left(\frac{1+\beta^2}{\alpha}+\beta\right)^2 = \frac{\beta^2+1}{\alpha}\left(\alpha+\beta+\frac{\beta^2+1}{\alpha}+\beta\right) \tag{5.3.21}$$

and therefore represent $g(\mathbf{z})$ as

$$g(\mathbf{z}) = L_0^2(\beta^2+1)\left(\frac{\partial}{\partial z_1}-\frac{\partial}{\partial z_2}\right)\left[e^{i\beta(z_1-z_2)}\Phi(z_1,z_2)\right], \tag{5.3.22}$$

which can be verified by simple differentiation.

One can derive a similar expression for the functions $\phi_1(\mathbf{z})$,

$$\phi_1(\mathbf{z}) \approx L_0\frac{e^{i\beta(z_1-z_2)}}{\pi}\int_{-\infty}^{\infty} e^{iz_1\alpha - iz_2\frac{\beta^2+1}{\alpha}}d\alpha = L_0 e^{i\beta(z_1-z_2)}\frac{\partial}{\partial z_1}\Phi(z_1,z_2), \tag{5.3.23}$$

and $\phi_2(\mathbf{z})$,

$$\begin{aligned}\phi_2(\mathbf{z}) &\approx L_0\frac{e^{i\beta(z_1-z_2)}}{\pi}\int_{-\infty}^{\infty}e^{iz_1\alpha-iz_2\frac{\beta^2+1}{\alpha}}\left(1+\left(\frac{1+\beta^2}{\alpha}+\beta\right)^2\right)\frac{d\alpha}{(\alpha+\beta)^2+1}\\ &= L_0\frac{e^{i\beta(z_1-z_2)}}{\pi}\int_{-\infty}^{\infty}e^{iz_1\alpha-iz_2\frac{\beta^2+1}{\alpha}}\frac{(\beta^2+1)d\alpha}{\alpha^2}\\ &= -L_0e^{i\beta(z_1-z_2)}\frac{\partial}{\partial z_2}\Phi(z_1,z_2),\end{aligned}\tag{5.3.24}$$

which again can be easily verified by the differentiation of the expression for $\Phi(z_1,z_2)$, Eq. (5.3.12).

5.3.3 The result

Now we have all necessary ingredients for evaluating the integral in Eq. (5.3.3). Substituting the expression for $g(\mathbf{z})$, Eq. (5.3.22), into the first half of the integral and integrating it by parts we obtain

$$\begin{aligned}\int\frac{d\mathbf{z}}{4\pi^2}Bf^{B-1}g &= BL_0^2\int\frac{d\mathbf{z}}{4\pi^2}f^{B-1}(\beta^2+1)\left(\frac{\partial}{\partial z_1}-\frac{\partial}{\partial z_2}\right)\left[e^{i\beta(z_1-z_2)}\Phi\right]\\ &= -BL_0^2\int\frac{d\mathbf{z}}{4\pi^2}(\beta^2+1)e^{i\beta(z_1-z_2)}\Phi\left(\frac{\partial}{\partial z_1}-\frac{\partial}{\partial z_2}\right)\left[f^{B-1}(\mathbf{z})\right]\\ &= B(B-1)L_0^2\int\frac{d\mathbf{z}}{4\pi^2}(\beta^2+1)f^{B-2}e^{2i\beta(z_1-z_2)}\Phi^2,\end{aligned}\tag{5.3.25}$$

and, gathering everything together,

$$R_2(x)=\frac{B(B-1)L_0^2}{\bar{d}^2}\int\frac{d\mathbf{z}}{4\pi^2}f^{B-2}e^{2i\beta(z_1-z_2)}\left[(\beta^2+1)\Phi^2-\frac{\partial\Phi}{\partial z_1}\frac{\partial\Phi}{\partial z_2}\right].\tag{5.3.26}$$

Now we need to take the limit $B\to\infty$. To do so we write $f^{B-2}(\mathbf{z})=e^{(B-2)\ln f}$ and rescale $f(\mathbf{z})$

$$f(\mathbf{u}/\beta)=e^{-\frac{|u_1+u_2|}{\beta}}-\frac{1}{\beta}\int_0^{u_1}e^{i(2y-u_1-u_2)}\Psi(y,u_1+u_2-y)dy\tag{5.3.27}$$

Thus, to the leading order in $1/\beta=\pi x/B$, we have

$$\begin{aligned}(B-2)\ln f(\mathbf{u}) &\approx -\pi x\left(|u_1+u_2|+\int_0^{u_1}e^{i(2y-u_1-u_2)}\Psi(y,u_1+u_2-y)dy\right)\\ &\equiv -\pi xQ\end{aligned}\tag{5.3.28}$$

where Ψ is the rescaled function Φ,

$$\Psi(\mathbf{u}) = \Phi\left(\frac{\mathbf{u}}{\beta}\right) = 2\,\mathrm{sign}(u_1)H(-u_1u_2)J_0\left(2\sqrt{-u_1u_2}\right), \tag{5.3.29}$$

and we have taken the limit $B \to \infty$ ($\beta \to \infty$).

Renormalising the rest of the Eq. (5.3.26) and taking the limit $B \to \infty$ we obtain

$$R_2(x) = \frac{1}{4}\int d\mathbf{u} e^{-\pi x Q} e^{2i(u_1-u_2)}\left[\Psi^2 - \frac{\partial\Psi}{\partial u_1}\frac{\partial\Psi}{\partial u_2}\right]. \tag{5.3.30}$$

For the derivatives of the function Ψ one has

$$\frac{\partial\Psi}{\partial u_1} = 2\left(J_0(0)\delta(u_1) + \mathrm{sign}(u_1)H(-u_1u_2)\frac{u_2 J_0'(2\sqrt{-u_1u_2})}{\sqrt{-u_1u_2}}\right), \tag{5.3.31}$$

$$\frac{\partial\Psi}{\partial u_2} = 2\left(-J_0(0)\delta(u_2) + \mathrm{sign}(u_1)H(-u_1u_2)\frac{u_1 J_0'(2\sqrt{-u_1u_2})}{\sqrt{-u_1u_2}}\right), \tag{5.3.32}$$

therefore, using $J_0(0) = 1$ and $J_0'(x) = -J_1(x)$,

$$\frac{\partial\Psi}{\partial u_1}\frac{\partial\Psi}{\partial u_2} = -4\left(\delta(u_1)\delta(u_2) + H(-u_1u_2)J_1(2\sqrt{-u_1u_2})\right). \tag{5.3.33}$$

Thus

$$R_2(x) = 1 + \int e^{-\pi x M + 2i(u_1-u_2)}\left[J_0^2(2\sqrt{-u_1u_2}) + J_1^2(2\sqrt{-u_1u_2})\right]H(-u_1u_2)d\mathbf{u}. \tag{5.3.34}$$

Now we perform the change of variables $u_2 \mapsto -u_2$ arriving to the integral representation of the two-point correlation function,

$$R_2(x) = 1 + \int_D e^{-\pi x M(\mathbf{u}) + 2i(u_1+u_2)}\left[J_0^2(2\sqrt{u_1u_2}) + J_1^2(2\sqrt{u_1u_2})\right]d\mathbf{u}, \tag{5.3.35}$$

where the domain of integration D includes first and third quarters of the $\mathbf{R}^2$ and $M(\mathbf{u})$ is given by

$$M(\mathbf{u}) \equiv M(u_1,u_2) = |u_1-u_2| + \int_0^{u_1} e^{i(2y-u_1+u_2)}\Psi(y, u_1-u_2-y)dy. \tag{5.3.36}$$

5.3.4 Properties of the function $M(\mathbf{u})$

In the subsequent material the function $M(\mathbf{u})$ plays an important role. We holds the key to both the asymptotic expansion of the two-point correlation function and the study of the singularities of the form factor. We begin by deriving the power series representation of $M(\mathbf{u})$.

We only need to consider the function $M(\mathbf{u})$ in the region $u_1 u_2 > 0$. Let us start with $u_1, u_2 > 0$. Then

$$M(\mathbf{u}) = |u_1 - u_2| + 2\int_0^{u_1} e^{i(2y-u_1+u_2)} H\left(y(y-u_1+u_2)\right) J_0\left(2\sqrt{y(y-u_1+u_2)}\right) dy. \quad (5.3.37)$$

Due to the presence of the Heaviside function H we need to consider two cases. If $u_2 > u_1$ then $y(y-u_1+u_2) \geq 0$ for any $y\colon 0 \leq y \leq u_1$ and therefore

$$M(\mathbf{u}) = u_2 - u_1 + 2\int_0^{u_1} e^{i(2y-u_1+u_2)} J_0\left(2\sqrt{y(y-u_1+u_2)}\right) dy. \quad (5.3.38)$$

In the case $u_1 > u_2$, however, the lower limit of the integration changes,

$$M(\mathbf{u}) = u_1 - u_2 + 2\int_{u_1-u_2}^{u_1} e^{i(2y-u_1+u_2)} J_0\left(2\sqrt{y(y-u_1+u_2)}\right) dy. \quad (5.3.39)$$

To find an expression which is valid for both regions, we calculate the integral

$$\int_0^{u_1-u_2} e^{i(2y-u_1+u_2)} J_0\left(2\sqrt{y(y-u_1+u_2)}\right) dy. \quad (5.3.40)$$

For simplicity we denote $u_1 - u_2 = b$ and write

$$e^{i(2y-b)} J_0\left(2\sqrt{y(y-b)}\right) = \Theta(y, y-b), \quad (5.3.41)$$

where

$$\begin{aligned}\Theta(x,y) \equiv e^{i(x+y)} J_0\left(2\sqrt{xy}\right) &= \sum_{j,k=0}^{\infty} \frac{i^{j+k} x^j y^k}{(j+k)!} \binom{j+k}{j} \sum_{n=0}^{\infty} (-1)^n \frac{x^n y^n}{n!n!} \\ &= \sum_{r,s=0}^{\infty} x^r y^s \sum_{n=0}^{\min(r,s)} \frac{(-1)^n i^{r+s-2n}}{n!n!(r-n)!(s-n)!} = \sum_{r,s=0}^{\infty} i^{r+s} \frac{x^r y^s}{r!s!} \sum_{n=0}^{\infty} \binom{r}{n}\binom{s}{n} \\ &= \sum_{r,s=0}^{\infty} i^{r+s} \binom{r+s}{r} \frac{x^r y^s}{r!s!}. \quad (5.3.42)\end{aligned}$$

Here we used the identity

$$\sum_{n=0}^{\infty} \binom{r}{n}\binom{s}{n} = \binom{r+s}{r}. \tag{5.3.43}$$

Now we substitute $x = y - b$ and integrate the series, remembering that

$$\int_0^b (y-b)^r y^s dy = (-1)^r \frac{r!s!}{(r+s+1)!} b^{r+s+1}, \tag{5.3.44}$$

see also Eq. (4.6.7). We obtain

$$\begin{aligned} \int_0^b \Theta(y, y-b)dy &= \sum_{r,s=0}^{\infty} \frac{i^{r+s} b^{r+s+1}}{(r+s+1)!}(-1)^r \binom{r+s}{r} \\ &= \sum_{r+s=0}^{\infty} \frac{i^{r+s} b^{r+s+1}}{(r+s+1)!}\delta_{r+s,0} = b. \end{aligned} \tag{5.3.45}$$

Thus, adding and subtracting $2b$ from Eq. (5.3.39), we can show that (5.3.38) is valid for both $u_2 > u_1$ and $u_1 > u_2$.

We remember that the function $f(\mathbf{u})$ which gave rise to $M(\mathbf{u})$ in our calculation in the previous Section satisfied a linear partial differential equation of the first order. Calculating partial derivatives of $M(\mathbf{u})$,

$$\frac{\partial M}{\partial u_1} = -1 + 2\int_0^{u_1} \frac{\partial}{\partial u_1}\Theta(y, y-u_1+u_2)dy + 2\Theta(u_1, u_2), \tag{5.3.46}$$

$$\begin{aligned} \frac{\partial M}{\partial u_2} &= 1 + 2\int_0^{u_1} \frac{\partial}{\partial u_2}\Theta(y, y-u_1+u_2)dy \\ &= 1 - 2\int_0^{u_1} \frac{\partial}{\partial u_1}\Theta(y, y-u_1+u_2)dy, \end{aligned} \tag{5.3.47}$$

we see that $M(\mathbf{u})$ also satisfies a PDE,

$$\frac{\partial M}{\partial u_1} + \frac{\partial M}{\partial u_2} = 2\Theta(u_1, u_2). \tag{5.3.48}$$

The initial condition can be easily supplied by substituting $u_1 = 0$:

$$M(0, u_2) = u_2. \tag{5.3.49}$$

Now we can find the series expansion of $M(\mathbf{u})$ by solving Eq. (5.3.48) with the initial condition (5.3.49). Writing

$$M(\mathbf{u}) = \sum_{j,k=0}^{\infty} A_{j,k} u_1^j u_2^k, \tag{5.3.50}$$

and denoting by $B_{j,k}$ the coefficients of the expansion of $2\Theta(u_1, u_2)$, as given by Eq. (5.3.42), we arrive to the recursion

$$A_{j+1,k} = \frac{1}{j+1}\left(B_{j,k} - (k+1)A_{j,k+1}\right), \qquad A_{0,k} = \delta_{0,k}. \tag{5.3.51}$$

This recursion is satisfied by $A_{1,0} = A_{0,1} = 1$ and

$$A_{j,k} = -2i^{j+k+1}\frac{(j+k-2)!}{j!k!(j-1)!(k-1)!}. \tag{5.3.52}$$

Indeed,

$$\begin{aligned}\frac{1}{j+1}\left(B_{j,k} - (k+1)A_{j,k+1}\right) &= \frac{2i^{j+k}}{(j+1)!k!}\left(\binom{j+k}{k} - \binom{j+k-1}{k}\right) \\ &= \frac{-2i^{j+k+2}}{(j+1)!k!}\binom{j+k-1}{j} = A_{j+1,k}. \end{aligned} \tag{5.3.53}$$

Thus for $u_1, u_2 > 0$

$$M(\mathbf{u}) = u_1 + u_2 - 2i\sum_{r,s=1}^{\infty}\frac{(iu_1)^r(iu_2)^s(r+s-2)!}{r!s!(r-1)!(s-1)!}. \tag{5.3.54}$$

Comparing the expansions for the functions $M(\mathbf{u})$ and $\Theta(\mathbf{u})$ we notice that they are quite similar. In fact,

$$\frac{\partial^2 M}{\partial u_1 \partial u_2}(\mathbf{u}) = 2i\Theta(\mathbf{u}). \tag{5.3.55}$$

An analysis, similar to the one presented in the pages above, of the function $M(\mathbf{u})$ in the region $u_1, u_2 < 0$ yields the PDE

$$\frac{\partial M}{\partial u_1} + \frac{\partial M}{\partial u_2} = -2\Theta(u_1, u_2), \qquad M(0, u_2) = -u_2. \tag{5.3.56}$$

Solving this PDE using the same methods we arrive to the general formula for $M(\mathbf{u})$,

$$M(\mathbf{u}) = |u_1| + |u_2| - 2i\,\mathrm{sign}(u_1)\sum_{r,s=1}^{\infty}\frac{(iu_1)^r(iu_2)^s(r+s-2)!}{r!s!(r-1)!(s-1)!}. \tag{5.3.57}$$

While we are at it, we might as well derive an expansion for the second factor in the integrand of representation (5.3.35) of the two-point correlation

function, the sum of the Bessel functions, $J_0^2(2\sqrt{-u_1u_2}) + J_1^2(2\sqrt{-u_1u_2})$. To derive it we use the standard formula (see, e.g. [41])

$$J_\nu(z)J_\mu(z) = (\frac{z}{2})^{\nu+\mu} \sum_{k=0}^{\infty} \frac{(-1)^k \Gamma(\nu+\mu+2k+1)(z/2)^{2k}}{\Gamma(\nu+k+1)\Gamma(\mu+k+1)\Gamma(\nu+\mu+k+1)k!}. \tag{5.3.58}$$

Applying this formula to our case, with $\nu = \mu = 0$ and $\nu = \mu = 1$, we obtain

$$\begin{aligned} J_0^2(2\sqrt{-u_1u_2}) + J_1^2(2\sqrt{-u_1u_2}) & \\ = \sum_{k=0}^{\infty} \frac{(-1)^k (2k)! u_1^k u_2^k}{k!k!k!k!} - \sum_{k=1}^{\infty} \frac{(-1)^k (2k)! u_1^k u_2^k}{k!k!(k+1)!(k-1)!} & \\ = 1 + \sum_{k=1}^{\infty} \frac{(-1)^k (2k)! u_1^k u_2^k}{k!k!} \left(\frac{1}{k!k!} - \frac{1}{(k+1)!(k-1)!} \right) & \\ = \sum_{k=0}^{\infty} \frac{(-1)^k (2k)! u_1^k u_2^k}{k!k!(k+1)!k!} & \end{aligned} \tag{5.3.59}$$

5.4 Expansion for large x

To derive an expansion of the two point correlation function $R_2(x)$ for large x we notice that since $M(-\mathbf{u}) = \overline{M(\mathbf{u})}$, the integral over the third quarter-plane in Eq. (5.3.35) is equal to the complex conjugate of the integral over second quarter-plane, i.e.

$$R_2(x) = 1 + 2\Re \int\int_0^{\infty} e^{-\pi x M(\mathbf{u}) + 2i(u_1+u_2)} J(\mathbf{u}) d\mathbf{u}, \tag{5.4.1}$$

where

$$J(\mathbf{u}) = J_0^2(2\sqrt{u_1u_2}) + J_1^2(2\sqrt{u_1u_2}) = \sum_{n=0}^{\infty} \frac{(-1)^n u_1^n u_2^n (2n)!}{(n+1)!(n!)^3}. \tag{5.4.2}$$

Now we can use the expansion of $M(\mathbf{u})$, Eq. (5.3.57), to expand $R_2(x)$ in the powers of $1/x$. We substitute $u_i = \gamma_i/(x\pi)$ and obtain

$$\begin{aligned} R_2(x) &= 1 + 2\Re \frac{1}{x^2\pi^2} \int\int_0^{\infty} d\gamma_1 d\gamma_2 e^{-\gamma_1-\gamma_2} \left[1 + \frac{2i\,(\gamma_1+\gamma_2-\gamma_1\gamma_2)}{x\pi} \right. \\ &\quad \left. - \frac{(5\gamma_1\gamma_2 + 2\gamma_1^2 + 2\gamma_2^2 - 5\gamma_1\gamma_2^2 - 5\gamma_1^2\gamma_2 + 2\gamma_1^2\gamma_2^2)}{x^2\pi^2} + O\left(\frac{1}{x^3}\right) \right] \\ &= 1 + 2\Re \left[\frac{1}{x^2\pi^2} + \frac{2i}{x^3\pi^3} - \frac{1}{x^4\pi^4} + \dots \right]. \end{aligned} \tag{5.4.3}$$

To compare it to the expansion of the form factor $K(\tau)$ we remember that the expansion of $R_2(x)$ in powers of $1/x$ and the expansion of $K(\tau)$ in powers of τ are connected through the Fourier transform: if $K(\tau) = 1 + \sum_{k=1}^{\infty} a_k \tau^k$ for $\tau > 0$ and $K(-\tau) = K(\tau)$ then

$$\begin{aligned} R_2(x) - 1 &= \delta(x) + 2\Re \lim_{\epsilon \to 0} \int_0^\infty (K(\tau) - 1) e^{-i2\pi(x - i\epsilon)\tau} d\tau \\ &= \delta(x) + 2\Re \lim_{\epsilon \to 0} \sum_{k=1}^{\infty} a_k \int_0^\infty \tau^k e^{-i2\pi(x - i\epsilon)\tau} d\tau \\ &= \delta(x) + 2\Re \sum_{k=1}^{\infty} \left(\frac{-i}{2\pi}\right)^{k+1} \frac{a_k k!}{x^{k+1}}. \end{aligned} \tag{5.4.4}$$

Applying this rule to

$$K(\tau) = 1 - 4\tau + 8\tau^2 - \frac{8}{3}\tau^3 + O(\tau^4), \tag{5.4.5}$$

we see that the first few coefficients of the both expansions agree.[1] In fact, it is possible to prove a much more general result, due to Bogomolny (also reported in [42])

Theorem 2. *Asymptotic expansion (5.4.1) of the two-point correlation function and expansion (3.1.42) for the form factor agree under Fourier transform,*

$$\int\!\!\int_0^\infty e^{-\pi x M(\mathbf{u}) + 2i(u_1 + u_2)} J(\mathbf{u}) d\mathbf{u} = \int_0^\infty (K(\tau') - 1)\, e^{-2\pi i x \tau'} d\tau'. \tag{5.4.6}$$

Proof. When taking the Fourier transform in Eq. (5.4.6), we give x a small imaginary part and then take limit as done in Eq.(5.4.4). This establishes the correspondence between the terms in the asymptotic expansion of

$$\widetilde{R_2}(x) = \int\!\!\int_0^\infty e^{-\pi x M(\mathbf{u}) + 2i(u_1 + u_2)} J(\mathbf{u}) d\mathbf{u} \tag{5.4.7}$$

and the terms of the small τ expansion of $K(\tau)$. This correspondence is

$$\frac{1}{(2\pi i x)^k} \longleftrightarrow \frac{\tau^{k-1}}{(k-1)!}. \tag{5.4.8}$$

[1] $\delta(x)$ is not present in the expansion Eq. (5.4.3), since the large x expansion "does not know" about the localised delta function.

Our plan is to modify the integrand in the definition of $\widetilde{R_2}(x)$, getting rid of the factor $e^{2i(u_1+u_2)}J(\mathbf{u})$, expand the integral in the inverse powers of x and apply the correspondence rule (5.4.8) recovering expansion (3.1.42).

First of all, let us derive a series expansion for

$$\Theta_1(\mathbf{u}) = -2i\sqrt{u_1u_2}J_1\left(2\sqrt{u_1u_2}\right)e^{i(u_1+u_2)}. \tag{5.4.9}$$

One way to do it is to relate $\Theta_1(\mathbf{u})$ to the function $\Theta(\mathbf{u}) = e^{i(u_1+u_2)}J_0\left(2\sqrt{u_1u_2}\right)$, expansion for which we know, see Eq. (5.3.42). We have

$$\begin{aligned}\frac{\partial}{\partial\mu}\Theta(\mu x,\mu y) &= i(x+y)\Theta(\mu x,\mu y) - 2\sqrt{\mu^2xy}J_1\left(2\mu\sqrt{xy}\right)e^{i\mu(x+y)}\\ &= x\frac{\partial\Theta}{\partial u_1}(\mu x,\mu y) + y\frac{\partial\Theta}{\partial u_2}(\mu x,\mu y),\end{aligned} \tag{5.4.10}$$

where $\partial\Theta/\partial u_i$ denotes the derivative of Θ with respect to ith argument. Hence we have for $\Theta_1(\mathbf{u})$

$$\Theta_1(\mathbf{u}) = i\left(u_1\frac{\partial}{\partial u_1}\Theta(\mathbf{u}) + u_2\frac{\partial}{\partial u_2}\Theta(\mathbf{u})\right) + (u_1+u_2)\Theta(\mathbf{u}). \tag{5.4.11}$$

Substituting the series expansion of the function $\Theta(\mathbf{u})$ into the above equation we obtain for the coefficient of the $u_1^ru_2^s$ term of the function $\Theta_1(\mathbf{u})$,

$$\begin{aligned}i^{r+s+1}\frac{(r+s)(r+s)!}{r!s!r!s!} + i^{r+s-1}\frac{(r+s-1)!}{((r-1)!s!)^2} + i^{r+s-1}\frac{(r+s-1)!}{(r!(s-1)!)^2}\\ = 2i^{r+s+1}\frac{(r+s-1)!}{r!s!(r-1)!(s-1)!},\end{aligned} \tag{5.4.12}$$

for $r,s>0$. Now we notice that the general terms of the expansions of the functions $M(\mathbf{u})$ and $\Theta_1(\mathbf{u})$ are very similar, the only difference being the factor $-(r+s-1)$ in the expansion of $\Theta_1(\mathbf{u})$. One of the ways to relate $M(\mathbf{u})$ to $\Theta_1(\mathbf{u})$ is to write

$$\frac{\partial}{\partial x}\left(xM\left(\frac{\alpha_1}{x},\frac{\alpha_2}{x}\right)\right) = \Theta_1\left(\frac{\alpha_1}{x},\frac{\alpha_2}{x}\right). \tag{5.4.13}$$

This is the first of the identities we will need. The second one is a modification of Eq. (5.3.48),

$$\left(\frac{\partial}{\partial\alpha_1}+\frac{\partial}{\partial\alpha_2}\right)\left(xM\left(\frac{\alpha_1}{x},\frac{\alpha_2}{x}\right)\right) = 2\Theta\left(\frac{\alpha_1}{x},\frac{\alpha_2}{x}\right). \tag{5.4.14}$$

Applying the first of the above identities we calculate

$$\frac{\partial^2}{\partial x^2} e^{-\pi x M\left(\frac{\alpha_1}{x},\frac{\alpha_2}{x}\right)} = e^{-\pi x M}\left(\pi^2\left(\frac{\partial}{\partial x}(xM)\right)^2 - \pi\frac{\partial^2}{\partial x^2}(xM)\right)$$
$$= e^{-\pi x M}\left(-4\pi^2\frac{\alpha_1\alpha_2}{x^2}J_1^2 e^{2\phi} - \frac{2\pi i}{x^3}\left(2J_0 e^{\phi}\alpha_1\alpha_2 + iJ_1 e^{\phi}\sqrt{\alpha_1\alpha_2}(\alpha_1+\alpha_2)\right)\right), \tag{5.4.15}$$

where $\phi = i(\alpha_1+\alpha_2)/x$ and the argument $(\alpha_1/x, \alpha_2/x)$ of the functions M, J_0, and J_1 is omitted.

Similarly using identity (5.4.14), we derive

$$\left(\frac{\partial}{\partial\alpha_1}+\frac{\partial}{\partial\alpha_2}\right)^2 e^{-\pi x M\left(\frac{\alpha_1}{x},\frac{\alpha_2}{x}\right)} = e^{-\pi x M}\left(\pi^2\Theta^2 - \pi\left(\frac{\partial}{\partial\alpha_1}+\frac{\partial}{\partial\alpha_2}\right)\Theta\right)$$
$$= e^{-\pi x M}\left(4\pi^2 J_0^2 e^{2\phi} - \frac{2\pi i}{\alpha_1\alpha_2 x}\left(2J_0 e^{\phi}\alpha_1\alpha_2 + iJ_1 e^{\phi}\sqrt{\alpha_1\alpha_2}(\alpha_1+\alpha_2)\right)\right) \tag{5.4.16}$$

Noticing the similarities of Eqs. (5.4.15) and (5.4.16) we subtract the first from the second, with the appropriate factors, to obtain

$$\frac{1}{4\pi^2}\left[\frac{1}{x^2}\left(\frac{\partial}{\partial\alpha_1}+\frac{\partial}{\partial\alpha_2}\right)^2 - \frac{1}{\alpha_1\alpha_2}\frac{\partial^2}{\partial x^2}\right] e^{-\pi x M\left(\frac{\alpha_1}{x},\frac{\alpha_2}{x}\right)}$$
$$= \frac{1}{x^2}\left[J_0^2+J_1^2\right]e^{2\phi}e^{-xM}, \tag{5.4.17}$$

where, as before, $\phi = i(\alpha_1+\alpha_2)/x$ and the argument $(\alpha_1/x, \alpha_2/x)$ is omitted after M, J_0 and J_1. The right hand side of Eq. (5.4.17) is exactly the integrand of Eq. (5.4.1) if we perform the change of variables $u_i = \alpha_i/x$ and therefore,

$$\widetilde{R_2}(x) = \iint_0^\infty \frac{d\alpha_1 d\alpha_2}{4\pi^2}\left[\frac{1}{x^2}\left(\frac{\partial}{\partial\alpha_1}+\frac{\partial}{\partial\alpha_2}\right)^2 - \frac{1}{\alpha_1\alpha_2}\frac{\partial^2}{\partial x^2}\right] e^{-\pi x M\left(\frac{\alpha_1}{x},\frac{\alpha_2}{x}\right)}. \tag{5.4.18}$$

The first summand in the integral can be evaluated as follows,

$$\iint_0^\infty \frac{d\alpha_1 d\alpha_2}{4\pi^2 x^2}\left(\frac{\partial}{\partial\alpha_1}+\frac{\partial}{\partial\alpha_2}\right)^2 e^{-\pi x M\left(\frac{\alpha_1}{x},\frac{\alpha_2}{x}\right)}$$
$$= \left(-2\pi\iint_0^\infty \frac{d\alpha_1 d\alpha_2}{4\pi^2 x^2}\left(\frac{\partial}{\partial\alpha_1}+\frac{\partial}{\partial\alpha_2}\right)\Theta e^{-\pi x M}\right)$$
$$= \left(-\int_0^\infty \frac{d\alpha_2}{2\pi x^2}\left[\Theta e^{-\pi x M}\right]_{\alpha_1=0}^{\infty} - \int_0^\infty \frac{d\alpha_1}{2\pi x^2}\left[\Theta e^{-\pi x M}\right]_{\alpha_2=0}^{\infty}\right). \tag{5.4.19}$$

Since

$$\left[\Theta\left(\frac{\alpha_1}{x},\frac{\alpha_2}{x}\right)e^{-\pi x M\left(\frac{\alpha_1}{x},\frac{\alpha_2}{x}\right)}\right]_{\alpha_1=0}^{\infty} = -e^{i\alpha_2/x}e^{-\pi\alpha_2}, \tag{5.4.20}$$

we obtain for the contribution of the first summand

$$\begin{aligned}\iint_0^\infty \frac{d\alpha_1 d\alpha_2}{4\pi^2 x^2}\left(\frac{\partial}{\partial\alpha_1}+\frac{\partial}{\partial\alpha_2}\right)^2 e^{-\pi x M\left(\frac{\alpha_1}{x},\frac{\alpha_2}{x}\right)} \\ = \left(\int_0^\infty \frac{d\alpha_2}{2\pi x^2}e^{i\alpha_2/x-\pi\alpha_2}+\int_0^\infty\frac{d\alpha_1}{2\pi x^2}e^{i\alpha_1/x-\pi\alpha_1}\right) \\ = \frac{1}{2\pi x^2}\frac{2}{\pi-i/x}.\end{aligned} \tag{5.4.21}$$

Now we can expand the answer in the inverse powers of x and apply the correspondence rule, Eq. (5.4.4). We obtain

$$\begin{aligned}\frac{1}{\pi x}\frac{1}{\pi x-i} &= -\sum_{k=0}^{\infty}\left(\frac{i}{\pi x}\right)^{k+2} \\ &= -\sum_{k=0}^{\infty}\frac{(-2)^{k+2}}{(2\pi i x)^{k+2}} \longleftrightarrow 2\sum_{k=0}^{\infty}\frac{(-2\tau)^{k+1}}{(k-1)!} = 2\left(e^{-2\tau}-1\right).\end{aligned} \tag{5.4.22}$$

Now we need to expand the second part of the integrand of Eq. (5.4.18),

$$\begin{aligned}\frac{\partial^2}{\partial x^2}e^{-\pi x M\left(\frac{\alpha_1}{x},\frac{\alpha_2}{x}\right)} &= \frac{\partial^2}{\partial x^2}e^{-\pi(\alpha_1+\alpha_2)}\exp\left(2\pi i\sum_{r,s=0}^{\infty}\frac{(i\alpha_1)^{r+1}(i\alpha_2)^{s+1}(r+s)!}{x^{r+s+1}r!s!(r+1)!(s+1)!}\right) \\ &= e^{-\pi(\alpha_1+\alpha_2)}\frac{\partial^2}{\partial x^2}\left[\sum_{j=0}^{\infty}\frac{(2\pi i)^j}{j!}\left(\sum_{r,s=0}^{\infty}\frac{(i\alpha_1)^{r+1}(i\alpha_2)^{s+1}(r+s)!}{x^{r+s+1}r!s!(r+1)!(s+1)!}\right)^j\right]\end{aligned} \tag{5.4.23}$$

Following notation (3.1.44) we expand the power j,

$$\begin{aligned}\left(\sum_{r,s=0}^{\infty}\frac{(i\alpha_1)^{r+1}(i\alpha_2)^{s+1}(r+s)!}{x^{r+s+1}r!s!(r+1)!(s+1)!}\right)^j &= \left(\sum_{r,s=0}^{\infty}\frac{(i\alpha_1)^{r+1}(i\alpha_2)^{s+1}}{x^{r+s+1}}F_1(r,s)\right)^j \\ &= \sum_{R,S=0}^{\infty}\frac{(i\alpha_1)^{R+j}(i\alpha_2)^{S+j}}{x^{R+S+j}}F_j(R,S),\end{aligned} \tag{5.4.24}$$

where, as in Chapter 3,

$$F_j(R,S) = \sum_{r_1+\ldots+r_j=R}\ \sum_{s_1+\ldots+s_j=S}\prod_{i=1}^{j}\frac{(r_i+s_i)!}{r_i!s_i!(r_i+1)!(s_i+1)!}, \tag{5.4.25}$$

i.e. $F_j(R,S)$ is the jth convolution of the infinite matrix $F_1(R,S)$ with itself. Continuing Eq. (5.4.23) we obtain

$$\frac{\partial^2}{\partial x^2} e^{-\pi x M\left(\frac{\alpha_1}{x},\frac{\alpha_2}{x}\right)} = e^{-\pi(\alpha_1+\alpha_2)} \sum_{j=1}^{\infty} \frac{(2\pi i)^j}{j!} \times \sum_{R,S=0}^{\infty} \frac{(R+S+j-1)!(i\alpha_1)^{R+j}(i\alpha_2)^{S+j}}{(R+S+j+1)!x^{R+S+j+2}} F_j(R,S). \quad (5.4.26)$$

Finally we integrate against $d\alpha_1 d\alpha_2/(4\pi^2\alpha_1\alpha_2)$ to arrive at

$$\begin{aligned} &-\iint_0^{\infty} \frac{d\alpha_1 d\alpha_2}{4\pi^2\alpha_1\alpha_2} \frac{\partial^2}{\partial x^2} e^{-\pi x M\left(\frac{\alpha_1}{x},\frac{\alpha_2}{x}\right)} \\ &= -\sum_{j=1}^{\infty} \frac{(2\pi i)^j}{4\pi^2 j!} \sum_{R,S=0}^{\infty} \frac{(R+S+j+1)!(R+j-1)!(S+j-1)!}{(R+S+j-1)!(-i\pi)^{R+S+2j}x^{R+S+j+2}} F_j(R,S) \\ &= \sum_{j=1}^{\infty} \frac{(-2)^j}{4j!} \sum_{R,S=0}^{\infty} \frac{(R+S+j+1)!(R+j-1)!(S+j-1)!}{(R+S+j-1)!(-i\pi x)^{R+S+j+2}} F_j(R,S) \\ &\longleftrightarrow \sum_{j=1}^{\infty} \frac{(-2)^j}{4j!} \sum_{R,S=0}^{\infty} \frac{(-2\tau)^{R+S+j+2}(R+j-1)!(S+j-1)!}{\tau(R+S+j-1)!} F_j(R,S) \\ &= \tau \sum_{j=1}^{\infty} \frac{(4\tau)^j}{j!} \sum_{R,S=0}^{\infty} \frac{(-2\tau)^{R+S}(R+j-1)!(S+j-1)!}{(R+S+j-1)!} F_j(R,S). \quad (5.4.27) \end{aligned}$$

This is exactly the same as the j sum in Eq. (3.1.42) with the exception of the extra $j=1$ term in the summation above. For $j=1$ we have

$$\begin{aligned} 4\tau^2 \sum_{R,S=0}^{\infty} \frac{(-2\tau)^{R+S} R!S!}{(R+S)!} F_j(R,S) &= \sum_{R,S=0}^{\infty} \frac{(-2\tau)^{R+S+2}}{(R+1)!(S+1)!} \\ &= \left(\sum_{R=0}^{\infty} \frac{(-2\tau)^{R+1}}{(R+1)!}\right)\left(\sum_{S=0}^{\infty} \frac{(-2\tau)^{S+1}}{(S+1)!}\right) = (1-e^{-2\tau})^2 \\ &= 1 - 2e^{-2\tau} + e^{-4\tau}, \quad (5.4.28) \end{aligned}$$

which together with the terms 1 and $2(e^{-2\tau}-1)$ gives the correct contribution $e^{-4\tau}$. □

5.5 Singularities of the form factor

It turns out that one can obtain some information about the singularities of $K(\tau)$ by studying integral representation (5.4.1). We are going to apply the

Fourier transform to the integral in Eq. (5.4.1) to recover the expansion of the form factor. There is, however, a subtle problem associated with this. The form factor is by definition an even function defined on the real line. What we want to get from transforming Eq. (5.4.1) is an analytic function which coincides with the form factor for real $\tau > 0$.

As we saw above,

$$\widetilde{R_2}(x) = \int\int_0^\infty e^{-\pi x M(\mathbf{u})+2i(u_1+u_2)} J(\mathbf{u}) d\mathbf{u} = \int_0^\infty (K(\tau')-1) e^{-2\pi i x\tau'} d\tau'. \tag{5.5.1}$$

Integrating (5.5.1) against $e^{2\pi i x\tau}$ on the real line (and thus effectively inverting the Fourier transform) we obtain

$$\int_{-\infty}^\infty \widetilde{R_2}(x) e^{2\pi i x\tau} dx = K(\tau) - 1, \qquad \tau > 0. \tag{5.5.2}$$

The left hand side can be viewed as the analytic continuation of the form factor restricted to $\tau > 0$ into the complex plane. Now we use $\widetilde{R_2}(-x) = \overline{\widetilde{R_2}(x)}$ to write

$$\int_{-\infty}^\infty e^{2\pi i x\tau} \widetilde{R_2}(x) dx = \int_0^\infty \left(e^{2\pi i x\tau} \widetilde{R_2}(x) + e^{-2\pi i x\tau} \overline{\widetilde{R_2}(x)} \right) dx$$

The only factor in the integral for $\widetilde{R_2}(x)$ which depends on x is $e^{-\pi x M(\mathbf{u})}$ and

$$\int_0^\infty e^{2\pi i x\tau} e^{-\pi x M(\mathbf{u})} dx = \frac{1}{\pi(M(\mathbf{u}) - 2i\tau)}, \tag{5.5.3}$$

thus we have for the form factor

$$K(\tau) = 1 + \frac{1}{\pi} \int\int_0^\infty \left[\frac{e^{2i(u_1+u_2)}}{M(\mathbf{u}) - 2i\tau} + \frac{e^{-2i(u_1+u_2)}}{\overline{M(\mathbf{u})} + 2i\tau} \right] J(\mathbf{u}) d\mathbf{u}. \tag{5.5.4}$$

The representation (5.5.4) presents us with a way to find the singularities of the form factor $K(\tau)$. They are given by the condition $\tau = M(\mathbf{u}_s)/(2i)$ and $\tau = \overline{M(\mathbf{u}_s)/(2i)}$, where the point $\mathbf{u}_s$ is such that

$$\frac{\partial M}{\partial u_1}(\mathbf{u}_s) = \frac{\partial M}{\partial u_2}(\mathbf{u}_s) = 0. \tag{5.5.5}$$

The derivative with respect to u_2 is

$$\frac{\partial M}{\partial u_2} = 1 - 2\int_0^{u_1} \left[e^{i(y+z)} J_1\left(2\sqrt{yz}\right)\sqrt{y/z} - ie^{i(y+z)} J_0\left(2\sqrt{yz}\right)\right] dy, \qquad (5.5.6)$$

where $z = y - u_1 + u_2$ and we assumed that $u_1 > u_2 > 0$. It is obvious from the expansion (5.3.57), however, that the function $M(\mathbf{u})$ is continuously differentiable if $u_1 u_2 > 0$ and that the expression (5.5.6) is valid for all $u_1 > 0$ and $u_2 > 0$. The expression in Eq. (5.5.6) is not easy to analyse and to simplify it we reduce our search to the values $u_2 = u_1$,

$$\frac{\partial M}{\partial u_2}(u_2 = u_1) = 1 - 2\int_0^{u_1} e^{2iy} J_1(2y)dy + 2i\int_0^{u_1} e^{2iy} J_0(2y)dy$$

Integrating the second integral by parts,

$$\int_0^{u_1} e^{2iy} J_0(2y)dy = \left.\frac{e^{2iy} J_0(2y)}{2i}\right|_0^{u_1} + \frac{2}{2i}\int_0^{u_1} e^{2iy} J_1(2y)dy, \qquad (5.5.7)$$

we obtain, after simplification,

$$\frac{\partial M}{\partial u_2}(u_2 = u_1) = e^{2iu_1} J_0(2u_1). \qquad (5.5.8)$$

Since $\frac{\partial M}{\partial u_1}(u_2 = u_1) = \frac{\partial M}{\partial u_2}(u_2 = u_1)$, the zeros of the derivatives of $M(\mathbf{u})$ on the line $u_2 = u_1$ are given by the zeros of the Bessel function J_0. The nearest zero is at $u_s \approx 1.202$. Then one of the poles of $K(\tau)$ is given by $\tau_s = M(1.202, 1.202)/(2i) = 0.462 - 0.420i$ which is in a very good agreement with the results of the numerical analysis. Although the numerical analysis is in favour of the claim that τ_s is the singularity nearest to the origin, we can prove it only partly.

Proposition 6. *Among the singularities arising from the values $u_2 = u_1$, the singularity at $\tau_s = M(1.202, 1.202)/(2i)$ is the nearest to the origin.*

Proof. To show that the statement is true we need to prove that the function $|M(u,u)|$ is growing with u. Indeed, on the line $u_1 = u_2$ the function$M$ is

$$M(u,u) = \int_0^{2u} e^{iy} J_0(y)dy = 2e^{2iu}u\left(J_0(2u) - iJ_1(2u)\right). \qquad (5.5.9)$$

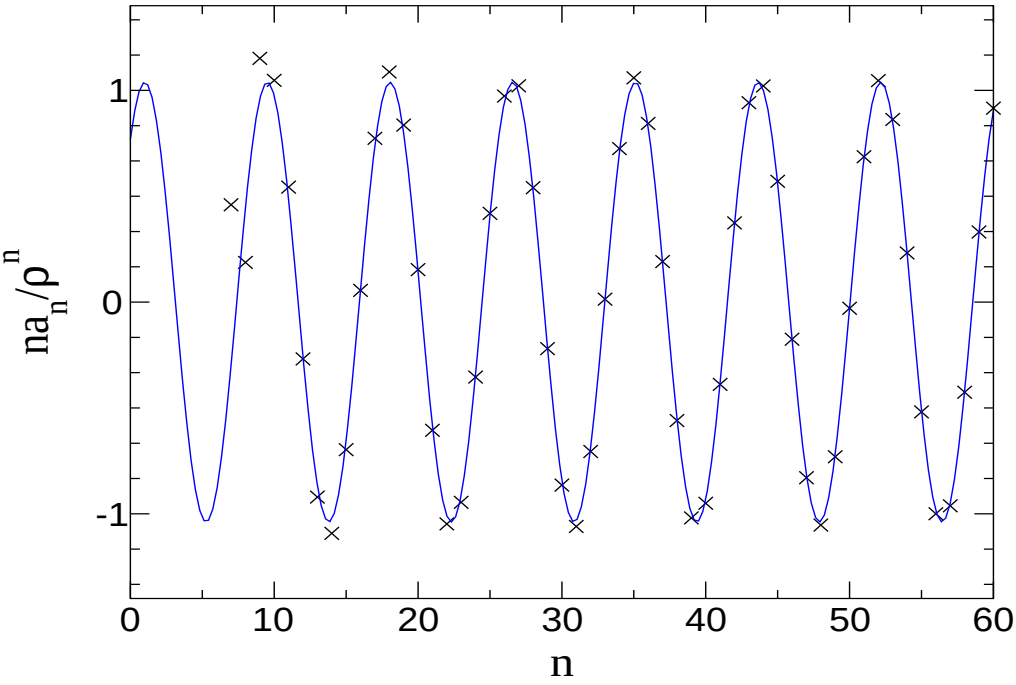

Figure 5.3: The coefficients of the power series expansion of $K(\tau)$ normalised by ρ^n (crosses) are compared to the prediction of Eq. (5.5.15). The fit gets better as n increases.

Then $|M(x/2, x/2)| = x^2 \left(J_0^2(x) + J_1^2(x)\right)$ and its derivative is (see [41])

$$\begin{aligned}
&\frac{d}{dx}|M(x/2,x/2)|^2 \\
&\quad = 2x\left(J_0^2(x)+J_1^2(x)\right) + x^2\big(-2J_0(x)J_1(x) + 2J_1(x)\left(J_0(x) - J_1(x)/x\right)\big) \\
&\qquad\qquad = 2xJ_0^2(x) \geq 0 \quad (5.5.10)
\end{aligned}$$

□

Further, one can approximate the behaviour of $K(\tau)$ near the singularities. Denoting a stationary point of $M(\mathbf{u})$ by $\mathbf{u}_s = (u_s, u_s)$, we expand

$$\begin{aligned}
M(\mathbf{u}) &\approx M(\mathbf{u}_s) + \frac{1}{2}\frac{\partial^2 M}{\partial u_1^2}(\mathbf{u}_s)(u_1-u_2)^2 + \frac{1}{2}\frac{\partial^2 M}{\partial u_2^2}(\mathbf{u}_s)(u_2-u_s)^2 \\
&\quad + \frac{\partial^2 M}{\partial u_1 \partial u_2}(\mathbf{u}_s)(u_1-u_s)(u_2-u_s) \\
&= M(\mathbf{u}_s) + \alpha_s\left((u_1-u_s)^2 + (u_2-u_s)^2\right), \qquad (5.5.11)
\end{aligned}$$

where, as we saw in Eq. (5.3.55), $\frac{\partial^2 M}{\partial u_1 \partial u_2}(\mathbf{u}_s) = e^{2iu_s}J_0(2u_s)/(2i)$ and is equal to zero since $\frac{\partial M}{\partial u_1}$ is equal to zero at $\mathbf{u}_s$. For the singularity associated with the

first Bessel zero, $\alpha_s = .385 - .349i$. Then the form factor

$$K(\tau) \approx \frac{1}{\pi\alpha_s} \iint_0^\infty \frac{J(\mathbf{u}) e^{2i(u_1+u_2)} d\mathbf{u}}{(u_1-u_s)^2 + (u_2-u_s)^2 + (M(\mathbf{u}_s) - 2i\tau)/\alpha_s} + \text{c.c.} \tag{5.5.12}$$

where the complex conjugate (c.c.) was taken pretending that τ is real. The main contribution to the integral comes from around the point $\mathbf{u}_s$. The integral near a singularity can be approximated by the value of the factor $J(\mathbf{u}) e^{\pm 2i(u_1+u_2)} / (\pi\alpha_s)$ at the singularity multiplied by

$$\iint_0 \frac{d\mathbf{u}}{u_1^2 + u_2^2 + \sigma} = \int_0^{2\pi} \int_0 \frac{r dr}{r^2 + \sigma} = \pi \int_0 \frac{dr^2}{r^2 + \sigma} = -\pi \ln \sigma, \tag{5.5.13}$$

where the absence of the upper limit indicates that the integral is taken in the vicinity of the lower limit. Thus we conclude that the leading order approximation of the form factor in the vicinity of the singularities (i.e. where σ, which corresponds to $M(\mathbf{u}_s) - 2i\tau$ or $\overline{M(\mathbf{u}_s)} + 2i\tau$, is small) is given by

$$K(\tau) \propto -C \ln\left(1 - \frac{2i\tau}{M(\mathbf{u}_s)}\right) - \overline{C} \ln\left(1 + \frac{2i\tau}{\overline{M(\mathbf{u}_s)}}\right), \tag{5.5.14}$$

where $C = J(\mathbf{u}_s) e^{4iu_s} / \alpha_s$. Expanding the contribution of Eq. (5.5.14) into the series around $\tau = 0$ we get

$$K(\tau) \propto 2\Re\left(C \sum_{n=1}^{\infty} \rho^n \frac{e^i n\phi}{n} \tau^n\right) = 2A \cos(\phi n + \psi) \frac{\rho^n}{n} \tau^n, \tag{5.5.15}$$

where $A = |J(\mathbf{u}_s) e^{4iu_s}/\alpha_s| \approx 0.519$, $\psi = \arg\left(J(\mathbf{u}_s) e^{4iu_s}/\alpha_s\right) \approx -0.737$, $\rho = |2i/M(\mathbf{u}_s)| \approx 1.602$ and $\phi = \arg\left(2i/M(\mathbf{u}_s)\right) \approx 0.737$. By Darboux Principle, the coefficients of expansion (5.5.15) should comprise the leading contribution to the exact coefficients given by Eqs. (3.1.42)-(3.1.43). To compare them we plot the exact coefficients na_n/ρ^n against the approximated coefficients $2A\cos(\phi n + \psi)$. The result is shown on Fig. 5.3.

5.6 Small x limit of $R_2(x)$

To derive an expression for $R_2(x)$ which is convenient in the limit of small x we return to Eq. (5.3.30). There we want to reexpress the term in the square

brackets in such a way that it is possible to do the integration by parts.

First of all, we notice that the properties of the Bessel functions imply that the function $\Psi(u)$ satisfies

$$\frac{\partial^2 \Psi}{\partial u_1 \partial u_2}(\mathbf{u}) = \Psi(\mathbf{u}). \tag{5.6.1}$$

Then, looking at the identities

$$\frac{\partial}{\partial u_1}\left(e^{2i(u_1-u_2)}\Psi^2\right) = 2ie^{2i(u_1-u_2)}\Psi^2 + 2e^{2i(u_1-u_2)}\Psi\frac{\partial \Psi}{\partial u_1}, \tag{5.6.2}$$

$$\frac{\partial}{\partial u_2}\left(e^{2i(u_1-u_2)}\Psi^2\right) = -2ie^{2i(u_1-u_2)}\Psi^2 + 2e^{2i(u_1-u_2)}\Psi\frac{\partial \Psi}{\partial u_2}, \tag{5.6.3}$$

and

$$\begin{aligned}
&\frac{\partial^2}{\partial u_1 \partial u_2}\left(e^{2i(u_1-u_2)}\Psi^2\right) \\
&\quad = e^{2i(u_1-u_2)}\left(4\Psi^2 + 4i\Psi\frac{\partial \Psi}{\partial u_2} - 4i\Psi\frac{\partial \Psi}{\partial u_1} + 2\frac{\partial \Psi}{\partial u_1}\frac{\partial \Psi}{\partial u_2} + 2\Psi\frac{\partial^2 \Psi}{\partial u_1 \partial u_2}\right) \\
&\quad = e^{2i(u_1-u_2)}\left(6\Psi^2 + 4i\Psi\frac{\partial \Psi}{\partial u_2} - 4i\Psi\frac{\partial \Psi}{\partial u_1} + 2\frac{\partial \Psi}{\partial u_1}\frac{\partial \Psi}{\partial u_2}\right),
\end{aligned} \tag{5.6.4}$$

we notice that

$$\begin{aligned}
&\left[\frac{\partial^2}{2\partial u_1 \partial u_2} + i\left(\frac{\partial}{\partial u_1} - \frac{\partial}{\partial u_2}\right)\right]\left(e^{2i(u_1-u_2)}\Psi^2\right) \\
&\qquad = e^{2i(u_1-u_2)}\left(\frac{\partial \Psi}{\partial z_1}\frac{\partial \Psi}{\partial z_2} - \Psi^2\right).
\end{aligned} \tag{5.6.5}$$

Substituting it into Eq. (5.3.30) and integrating by parts we obtain

$$\begin{aligned}
R_2(x) &= -\frac{1}{4}\int d\mathbf{u} e^{-\pi x Q}\left[\frac{\partial^2}{2\partial u_1 \partial u_2} + i\left(\frac{\partial}{\partial u_1} - \frac{\partial}{\partial u_2}\right)\right]\left(e^{2i(u_1-u_2)}\Psi^2(u_1,u_2)\right) \\
&= \int \frac{d\mathbf{u}}{4} e^{2i(u_1-u_2)}\Psi^2\left[i\left(\frac{\partial}{\partial u_1} - \frac{\partial}{\partial u_2}\right) - \frac{\partial^2}{2\partial u_1 \partial u_2}\right]\left(e^{-\pi x Q}\right).
\end{aligned} \tag{5.6.6}$$

Now, using the identities (compare to Eqs.(5.3.48) and (5.3.55))

$$\frac{\partial Q}{\partial u_1} - \frac{\partial Q}{\partial u_2} = e^{i(u_1-u_2)}\Psi, \qquad \frac{\partial^2 Q}{2\partial u_1 \partial u_2} = -ie^{i(u_1-u_2)}\Psi, \tag{5.6.7}$$

we write

$$\left[i\left(\frac{\partial}{\partial u_1}-\frac{\partial}{\partial u_2}\right)-\frac{\partial^2}{2\partial u_1\partial u_2}\right]\left(e^{-\pi x Q}\right)$$
$$=e^{-\pi x Q}\left(-i\pi x\left(\frac{\partial Q}{\partial u_1}-\frac{\partial Q}{\partial u_2}\right)+\frac{\pi x}{2}\frac{\partial^2 Q}{\partial u_1\partial u_2}-\frac{(\pi x)^2}{2}\frac{\partial Q}{\partial u_1}\frac{\partial Q}{\partial u_2}\right)$$
$$=-e^{-\pi x Q}\left(\frac{3i\pi x}{2}e^{i(u_1-u_2)}\Psi+\frac{(\pi x)^2}{2}\frac{\partial Q}{\partial u_1}\frac{\partial Q}{\partial u_2}\right). \quad (5.6.8)$$

Thus we finally obtain

$$R_2(x)=-\int\frac{d\mathbf{u}}{8}e^{-\pi x Q}e^{2i(u_1-u_2)}\Psi^2\left[\pi^2x^2\frac{\partial Q}{\partial u_1}\frac{\partial Q}{\partial u_2}+3i\pi x\Psi e^{i(u_1-u_2)}\right], \quad (5.6.9)$$

From Eq. (5.6.9) one can see that the two-point correlation function $R_2(x)$ is linear in x for small x and the corresponding numerical factor was computed in [32],

$$\begin{aligned}3i\pi\int e^{3i(u_1-u_2)}\Psi^3 d\mathbf{u} &= 3i\pi\int_D \mathrm{sign}(u_1)e^{3i(u_1-u_2)}J_0^3\left(2\sqrt{-u_1u_2}\right)du\\ &= 3i\pi\int_0^\infty\int_{-\infty}^0 e^{3i(u_1-u_2)}J_0^3\left(2\sqrt{-u_1u_2}\right)du_1du_2+\text{c.c.}\\ &= -\frac{\pi\sqrt{3}}{2}, \quad (5.6.10)\end{aligned}$$

producing

$$R_2(x)=\frac{\pi\sqrt{3}}{2}x+O(x^2). \quad (5.6.11)$$

5.7 Comparing star graphs and Šeba billiards

The original Šeba billiard, which is a rectangular billiard quantized and perturbed by a delta function, see Fig. 5.4, was introduced in [33] as an example of a system whose classical counterpart is integrable (the delta function affects only measure zero set of the orbits) but which nonetheless exhibits features of quantum chaos. This construction was later generalized to quantized versions of any integrable system [34] which retained the aforementioned properties. We will refer to any system in this class as a "Šeba billiard".

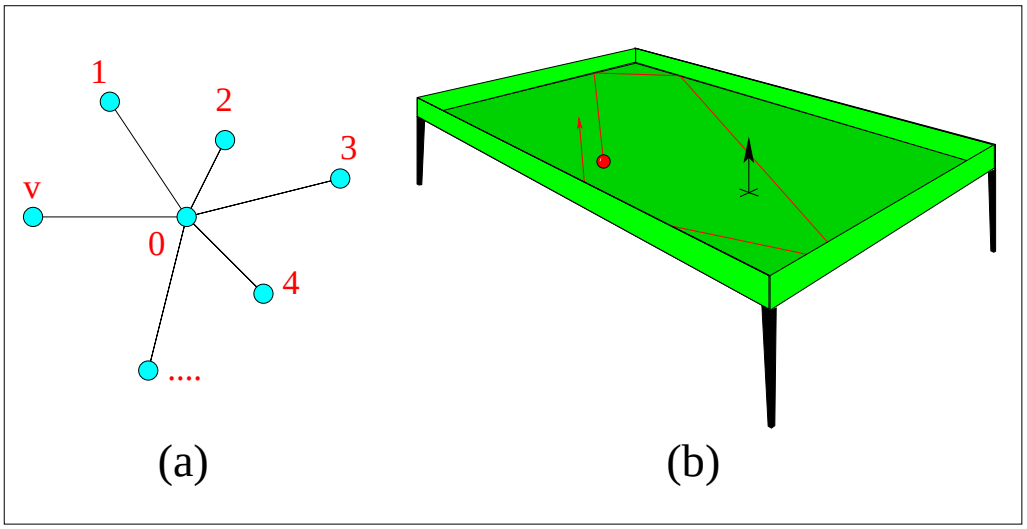

Figure 5.4: A star graph with v edges (a) and a Šeba billiard (b): different systems with the same statistics.

The energy levels of a Šeba billiard can be found by solving an explicit equation which depends on the levels of the original unperturbed system and on the boundary conditions imposed at the singularity. This equation takes the general form $\xi(z) = 0$, where $\xi(z)$ is a meromorphic function; for example, for one particular choice of boundary condition [33, 34]

$$\xi(z) = \sum_n \left(\frac{1}{E_n - z} - \frac{E_n}{E_n^2 + 1} \right), \tag{5.7.1}$$

where $\{E_i\}$ are the eigenlevels of the unperturbed system. Using this explicit expression and assuming that $\{E_i\}$ are given by a Poisson process, one can derive the associated functions such as the joint distribution of the levels of the Šeba billiard, asymptotics of the level spacing distribution [34] and the two-point spectral correlation function [32]. The results show the presence of the spectral correlations but are substantially different from RMT results.

The derivation presented above in the Sections 5.2, 5.3 and 5.6 is the result of the application of the methods developed in [32] to calculating $R_2(x)$ for the star graphs. Although concerning statistics of zeroes of two different functions, (5.1.3) and (5.7.1), both derivation follow the same route and, most importantly, produce exactly the same result.

The heuristic reasons for this somewhat surprising result are the following. First, the dynamics in both systems is centered around the single point scatterer. In the star graphs it is the central vertex and in the Šeba billiards it is the delta function. Furthermore, in between scatterings the dynamics is integrable in both cases.

The second reason is given by an application of the Mittag-Leffler theorem to the meromorphic function $\tan z$:

$$\tan z = \sum_{n=-\infty}^{\infty} \left(\frac{1}{n\pi + \pi/2 - z} - \frac{1}{n\pi + \pi/2} \right). \tag{5.7.2}$$

Thus we can rewrite Eq. (5.1.3) in the form similar to (5.7.1) and since the poles of the function in Eq. (5.1.3) in the limit $B \to \infty$ have properties similar to the ones of a Poisson sequence, it is less surprising that the two point correlation functions are the same.

Finally, we remark that the results of this Chapter demonstrate that, at least in the special case considered here, graphs are able to reproduce features of other, experimentally realizable, quantum systems, and also that they provide further confirmation that spectral statistics can be computed exactly using the trace formula as we have done in Chapter 3.

Appendix A

Combinatorial results

A.1 General properties of degeneracy classes

Theorem 3 (The number of the degeneracy classes). *Let G be a graph with V vertices and B (non-directed) bonds. Denote by $D(m)$ the number of the degeneracy classes of the period m. Then $D(2n)+D(2n+1)$ is a polynomial in n of order $B-1$ with the leading term*

$$2^{B-V+1}\frac{n^{B-1}}{(B-1)!}. \tag{A.1}$$

Proof. First we recall that the degeneracy classes can be labelled by the vectors $\mathbf{s} \in \mathbb{N}_0^B$ (c.f. Eq. (2.1.15) and Def. 6). However not all such vectors correspond to degeneracy classes. There are two restrictions. First, the "Euler condition", is

$$\sum_{j\,:\,(i,j)\in\mathcal{B}} s_{(i,j)} \qquad \text{is even for any } i \in \mathcal{V}, \tag{A.2}$$

where $s_{(i,j)}$ is the component of the vector $\mathbf{s}$ corresponding to the non-directed bond (i,j). The above condition arises from the fact that *passing* through the vertex i adds 2 to the sum in Eq. (A.2) and if the sum was odd it would mean that the orbits in the degeneracy class would "get stuck" at the vertex i.

The second restriction is the connectivity of the degeneracy class. For this restriction there is no convenient description in terms of the vector $\mathbf{s}$. However,

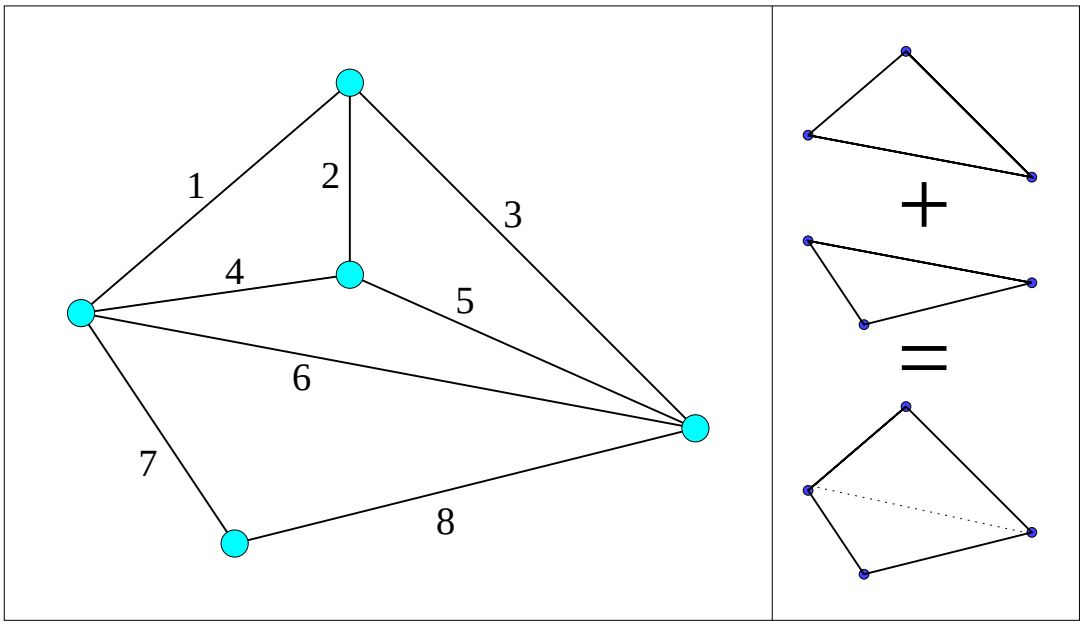

Figure A.1: On the left: an example of a graph. On the right: addition of two skeletons. The dotted bond disappears after the addition.

as we shall see, the number of disconnected degeneracy classes is sub-dominant to the number of connected ones.

First we count all degeneracy classes, both connected and disconnected. That is, we count all vectors $\mathbf{s}$ satisfying Eq. (A.2). For a degeneracy class, the *skeleton* is the set of all bonds b such that s_b is odd. It is clear that the skeleton of a degeneracy class will satisfy Eq. (A.2) itself and will have the associated vector $\mathbf{s}_{sc} \in \mathbb{N}_0^B$ with the components equal to 1 corresponding to the bonds that are in the skeleton and zeros corresponding to the bonds that are not. Thus we decompose each vector $\mathbf{s}$ satisfying Eq. (A.2) into the sum

$$\mathbf{s} = \mathbf{s}_{sc} + \mathbf{s}_{fl}, \tag{A.3}$$

where the "flesh component" $\mathbf{s}_{fl}$ has only even components. Such a decomposition is clearly unique.

Now we want to count the number of all possible skeletons on our graph. Let Z_G denote the cycle space of the graph and let $\{z_i\}_{i=1}^{\dim Z_G}$ be a basis of the cycle space (see, e.g., [43]). For example, the dimension of the cycle space of the graph on Fig. A.1 is four and one of the possible choices of the basis

consists of the cycles $\{(1,3,6),(1,2,4),(2,3,5),(6,7,8)\}$. We define the sum of two cycles as a set which consists of all the bonds which belong to one of the summands but not to both (logical *excluding OR*). For example, the addition

$$(1,3,6)+(6,7,8)=(1,3,8,7) \tag{A.4}$$

is illustrated on Fig. A.1. Sum of more than two summands is defined by induction, like in

$$(1,3,6)+(1,2,4)+(2,3,5)=(2,3,6,4)+(2,3,5)=(4,5,6) \tag{A.5}$$

One can check that this operation is associative and that the result is always a skeleton. It is also true that any skeleton can be represented as a sum of some of the basis cycles with coefficients 0 or 1 in a unique way. Thus the number of all possible skeletons is equal to $2^{\dim Z_G}$ with the empty skeleton being one of them. It is a well-known result that the dimension of the cycle space is $\dim Z_G = B - V + 1$ (see, for example, [43]).

Now if we have a skeleton $\mathbf{s}_{sc}$ with $|\mathbf{s}_{sc}|$ "bones", we have to count all possible "flesh components" with the sum of the vector elements equal to $2n - |\mathbf{s}_{sc}|(+1)$, where 1 is added if $|\mathbf{s}_{sc}|$ is odd. It is the same as the number of ways to distribute $n - [|\mathbf{s}_{sc}|]$ couples of objects between B distinguishable bins. Here $[x]$ stands for the integer part of x. The answer to our question is the binomial coefficient

$$\binom{n-[|\mathbf{s}_{sc}|]+B-1}{B-1}, \tag{A.6}$$

which is a polynomial in n with the leading term given by $\frac{n^{B-1}}{(B-1)!}$, independent of $|\mathbf{s}_{sc}|$. Multiplying the leading term by the number of all skeletons we obtain the leading order approximation to the number of all degeneracy classes, connected and disconnected.

We can estimate from above the number of disconnected degeneracy classes by the number of all disconnected subgraphs of G multiplied by the number of all degeneracy classes that belong to the subgraph. But the number of the

subgraphs does not depend on n and the number of the degeneracy classes in a subgraph must have order less than $B-1$ since the subgraph has less bonds than the original graph. Thus the number of disconnected degeneracy classes is sub-dominant. □

Remark. If S_e is the number of all skeletons with even number of bones and S_o is the number of odd ones then

$$D(2n) \propto S_e \frac{n^{B-1}}{(B-1)!} \tag{A.7}$$

$$D(2n+1) \propto S_o \frac{n^{B-1}}{(B-1)!} \tag{A.8}$$

However it is better to consider the sum $D(2n)+D(2n+1)$ as it might happen that $S_o = 0$ (e.g. for star graphs). There is always at least one even skeleton — the empty one.

Theorem 4 (Upper bound on a degeneracy class contribution). *Given a degeneracy class* $\mathbf{s}$*, its contribution is bounded by*

$$\left| \sum_{\mathbf{s}(\mathbf{p})=\mathbf{s}} \frac{A_{\mathbf{p}}}{r_{\mathbf{p}}} \right| \leq 2B, \tag{A.9}$$

where B *is the number of bonds of the graph.*

Proof. We remind ourselves that the contribution of the degeneracy class $\mathbf{s}$ is the coefficient of $e^{ik\ell}$ in the expansion of $\mathrm{Tr}(\mathbf{DS})^n$, Eq. (2.3.16), where $\ell = \sum_{i=1}^{B} s_i L_i$.

Form the $2B \times 2B$ diagonal matrix $\mathbf{Z}$ with the elements $Z_{b,b} = z_b$, where z_b are complex variables, and identify the variables z_b and $z_{\overline{b}}$. Then if we put $z_i = e^{ikL_i}$, we will recover the matrix $\mathbf{D}$, Eq. (2.2.10).

The trace $\mathrm{Tr}(\mathbf{ZS})^n$ is a polynomial of degree n in B complex variables. The contribution of the degeneracy class $\mathbf{s}$ is given by the coefficient of $z_1^{s_1} z_2^{s_2} \cdots z_B^{s_B}$. The upper bound for such coefficient is given by the Cauchy inequality,

$$\left| \sum_{\mathbf{s}(\mathbf{p})=\mathbf{s}} \frac{A_{\mathbf{p}}}{r_{\mathbf{p}}} \right| \leq \max \left| \mathrm{Tr}(\mathbf{ZS})^n \right|, \tag{A.10}$$

where the maximum is taken over the variables z_i taking values on the unit circle, $z_i = e^{i\phi_i}$. However for such values of the variables the matrix $\mathbf{Z}$ is unitary thus $(\mathbf{ZS})^n$ is also unitary of dimension $2B \times 2B$ thus $\max |\mathrm{Tr}(\mathbf{ZS})^n| \leq 2B$. □

A.2 Partitions of an integer into a sum of non-zero summands

The number of partitions of the integer n into k non-zero summands is a well known combinatorial quantity. Rigorously speaking, it is the number of solutions in $\mathbb{N} = \{1, 2, 3, \dots\}$ of the equation

$$x_1 + x_2 + \cdots + x_k = n, \qquad x_i \in \mathbb{N}. \tag{A.1}$$

We denote such number by $b(n, k)$.

Let $(a_1, \dots, a_k)$ be such a solution. Then the set $\{a_1, a_1 + a_2, \dots, a_1 + \cdots + a_{k-1}\}$ consists of $k - 1$ numbers which are distinct, ordered, greater than 0 and less than n. In fact, the solutions of Eq. (A.1) are in one-to-one correspondence with such subsets of the set $\{1, \dots, n-1\}$: given an ordered subset $\{c_1, c_2, \dots, c_{k-1}\}$ we obtain a solution of Eq. (A.1) by setting $a_1 = c_1$, $a_2 = c_2 - c_1$, $\dots$, $a_{k-1} = c_{k-1} - c_{k-2}$, $a_k = n - c_{k-1}$. Thus the number of the solutions to Eq. (A.1) is equal to the number of all $k-1$-element subsets of $\{1, \dots, n-1\}$,

$$b(n, k) = \binom{n-1}{k-1}. \tag{A.2}$$

This number is extensively used in the present work which was the reason for the inclusion of its derivation.

A.3 Permutations without liaisons.

In this section we address one of the most important underlying questions of the present work. Given g_1 ordered objects of type 1, g_2 ordered objects of type

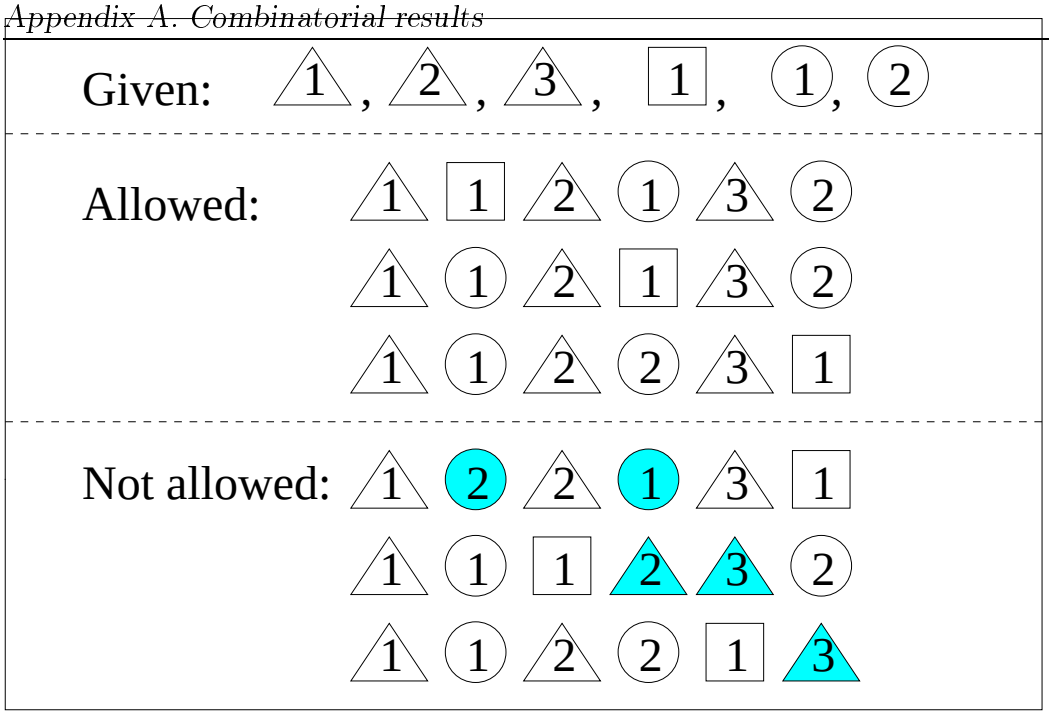

Figure A.2: Permutations that are allowed and not allowed. Different shapes correspond to the different types of objects: there are 3 types with $g_1 = 3$, $g_2 = 1$ and $g_3 = 2$. The three examples of the permutations that are not allowed violate conditions 2, 3 and 4 correspondingly. The offending objects are shaded.

2, ... , g_j ordered objects of type j, count the permutations of these objects which satisfy the following conditions,

1. First object of the type 1 comes first.
2. Order of the objects is preserved in the permutation.
3. No objects of the same type may stand next to each other.
4. The last object cannot be of the type 1.

We denote the answer to our question by $R_{g_1,\dots,g_j}$. This question is purely combinatorial and throughout this section we forget about the nature of the objects as groups of bonds.

Remark 4. Condition 4 may be considered to be a special case of condition 3, if we adopt the cyclic vision of the permutation.

For an example of permutations satisfying and not satisfying the above conditions, see Fig. A.2. Following the solution of a similar problem in [24], we address this problem using an inclusion-exclusion principle. Temporarily we forget about conditions 3 and 4 and consider all permutation satisfying the remaining conditions. If two objects of the same type stand next to each other we say that they form a *liaison*. Our ultimate goal is to count all permutation without liaisons.

Since condition 2 remains in force, only two consecutive objects of the same type can form a liaison. Thus there is maximum of $g_i - 1$ liaisons to be formed by the objects of the type i and $G - v$ possible liaisons altogether, where $G = \sum_{i=1}^{j} g_i$.

To count all permutation without liaisons we use the following inclusion-exclusion principle. Let X be a finite set and $\mathcal{P}$ be a finite set of boolean functions (properties) on X:

$$\forall p \in \mathcal{P} \qquad p\colon X \to \{0,1\}\,. \tag{A.1}$$

If p is a property then we denote by X_p the set of all x for which the property p holds, i.e. $p(x) = 1$. If P is a subset of $\mathcal{P}$, by X_P we denote the subset of X

$$X_P = \Big\{x \in X\colon\ (\forall p \in P)\,[p(x) = 1]\Big\} = \bigcap_{p\in P} X_p. \tag{A.2}$$

We also put $X_\emptyset = X$.

Proposition 7. *The number of elements in X which do not satisfy any properties from $\mathcal{P}$ is given by*

$$\left| X \setminus \bigcup_{p\in\mathcal{P}} X_p \right| = \sum_{P\subset\mathcal{P}} (-1)^{|P|}\,|X_P|\,, \tag{A.3}$$

where the modulus sign stands for the number of elements in the set and the sum is taken over all subsets of $\mathcal{P}$, including the empty set and the set $\mathcal{P}$ itself.

Proof. Eq. (A.3) is a slightly altered version of the more traditional inclusion-

exclusion principle

$$\left|\bigcup_{p\in\mathcal{P}} X_p\right| = \sum_{p\in\mathcal{P}} |X_p| - \sum_{p,q\in\mathcal{P}} |X_p \cap X_q| + \sum_{p,q,r\in\mathcal{P}} |X_p \cap X_q \cap X_r| - \dots , \quad \text{(A.4)}$$

which is obtained by iterating the formula

$$|A \cup B| = |A| + |B| - |A \cap B| . \quad \text{(A.5)}$$

□

If the properties $\mathcal{P}$ are such that $|X_P|$ depends only on $|P|$,

$$|X_P| = f(|P|) \quad \text{(A.6)}$$

then

$$\left|X \setminus \bigcup_{p\in\mathcal{P}} X_p\right| = \sum_{i=0}^{|\mathcal{P}|} (-1)^i \binom{|\mathcal{P}|}{i} f(i). \quad \text{(A.7)}$$

We now generalise Proposition 7 to j sets of properties

Proposition 8. *If there are j sets of properties, $\mathcal{P}_i$, $i = 1, \dots , j$, and*

$$X_{P_1,P_2,\dots,P_j} = \bigcap_{i=1}^{j} X_{P_i} \quad \text{(A.8)}$$

are such that

$$|X_{P_1,P_2,\dots,P_j}| = f(|P_1|, |P_2|, \dots , |P_j|) \quad \text{(A.9)}$$

then the number of elements in X which do not satisfy any of the properties is given by

$$\left|X \setminus \left(\bigcup_{i=1}^{j} \bigcup_{p\in\mathcal{P}_i} X_p\right)\right| = \sum_{l_1,l_2,\dots,l_j} (-1)^{l_1+\dots+l_j} f(l_1, l_2, \dots , l_j) \prod_{i=1}^{j} \binom{|\mathcal{P}_i|}{l_i}. \quad \text{(A.10)}$$

To apply Proposition 8 to our problem we define a set of properties on all possible permutation of object as follows: to each of the possible liaisons we associate a function which is equal to one on the permutations that contain such liaison and is zero otherwise. We group the properties by the type of the

liaison they are associated with. Thus we obtain j sets of properties, $G - j$ properties in total. The quantity we are seeking, the number of permutations without liaisons, is exactly the left-hand side of Eq. (A.10).

To make use of Eq. (A.10) we need to know the number $f(l_1, \ldots, l_v)$. The meaning of this number is as follows: fix l_1 liaisons of the first type, l_2 liaisons of the second type etc; how many permutations are there containing those fixed liaisons and, possibly, other liaisons as well. If $l_i = 0$ for all i (the situation with no restrictions) then it is not hard to see that $f(0, 0, \ldots, 0)$ is equal to the number of all permutations of $G - 1 = g_1 - 1 + g_2 + \ldots + g_j$ objects of j types with any two objects of the same type being indistinguishable. The minus one contribution is there because the position of one object of the first type is fixed, it must come first. The indistinguishability comes from the need to preserve the order of the objects of the same type: being ordered and being indistinguishable is equivalent in terms of combinatorics. Thus the answer for $f(0, 0, \ldots, 0)$ is

$$f(0, \ldots, 0) = \frac{(G-1)!}{(g_1 - 1)! g_2! \cdots g_v!}. \tag{A.11}$$

Let us now select l_1 liaisons among the objects of the type 1, l_2 liaisons among the objects of the type 2 and so forth, $0 \le l_i \le g_i - 1$. We can consider two or more objects bound together by liaison(s) to be a single object, its position in the ordering within its type being obvious. Now, by analogy with Eq. (A.11), we derive

$$f(l_1, \ldots, l_v) = \frac{(G - l_1 - \ldots - l_v - 1)!}{(g_1 - l_1 - 1)!(g_2 - l_2)! \cdots (g_v - l_v)!}. \tag{A.12}$$

Applying Proposition 8 we obtain the number of permutations without liaisons to be equal to

$$\sum_{l_1, \ldots, l_v} (-1)^{l_1 + \ldots + l_v} \frac{(G - l_1 - \ldots - l_v - 1)!}{(g_1 - l_1 - 1)!(g_2 - l_2)! \cdots (g_v - l_v)!} \prod_{i=1}^{v} \binom{g_i - 1}{l_i}. \tag{A.13}$$

There is one last detail to be fixed: nothing in our derivation prevents condition 4 from being violated. To mend it we consider the situation when this

condition is violated to be a special form of liaison, between the last group and the first group of "1". This way there are g_1 liaisons of type 1 to choose from and we should write $\binom{g_1}{l_1}$ instead of $\binom{g_1-1}{l_1}$. The rest of formula (A.13) remains unchanged. Performing change of variables $k_i = g_i - l_i$ we finally arrive to

$$R_{g_1,\ldots,g_v} = (-1)^G g_1 \sum_{k_1,\ldots,k_v} \frac{(-1)^{k_1+\ldots+k_v}}{k_1+\ldots+k_v} \binom{k_1+\ldots+k_v}{k_1,\ldots,k_v} \prod_{i=1}^{v} \binom{g_i-1}{k_i-1}, \tag{A.14}$$

where $G = \sum_{i=1}^{v} g_i$.

Appendix B

List of notations

$\binom{n}{k}$	binomial (for $n < k$ or $k < 0$ defined to be 0)
$[a, b, c]$	sequence
(a, b, c)	orbit
$\{a, b, c\}$	set
δ_{xy}	Kronecker delta (1 whenever $x = y$, 0 otherwise)
$\delta(x)$	Dirac delta function
$\lvert\mathbf{s}\rvert = \sum s_i$	if $\mathbf{s}$ is a vector
$\lvert\mathcal{S}\rvert$	number of elements in $\mathcal{S}$ if $\mathcal{S}$ is a set
$\mathbb{N}_0$	set of non-negative integers
$\Re z$	real part of z
$\Im z$	imaginary part of z
$\square$	end of proof (QED)

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