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Nodal counting on quantum graphs

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Abstract

We consider the real eigenfunctions of the Schrödinger operator on graphs, and count their nodal domains. The number of nodal domains fluctuates within an interval whose size equals the number of bonds B. For well connected graphs, with incommensurate bond lengths, the distribution of the number of nodal domains in the interval mentioned above approaches a Gaussian distribution in the limit when the number of vertices is large. The approach to this limit is not simple, and we discuss it in detail. At the same time we define a random wave model for graphs, and compare the predictions of this model with analytic and numerical computations.

1. Introduction—the Schrödinger operator on graphs

The structure of the nodal set of wavefunctions reflects the type of the underlying classical flow. This was suspected and discussed a long time ago, [1–4], and returned to the focus of current research once it was shown that not only the morphology, but the distribution of the *number* of nodal domains, is indicative of the nature of the underlying dynamics [5]. This was followed by several other studies of nodal statistics [6–10], and their relation to the random waves ensemble [11].

Quantum graphs are excellent paradigms of quantum chaos [12], and in this work we try to check to what extent the statistics of nodal domains in graphs follow the patterns observed in the study of wavefunctions of the Schrödinger operators in the typical systems (e.g., billiards) where quantum chaos is often discussed. Graphs are one-dimensional systems. Their complex features stem from the fact that they are not simply connected. Because of this fact, Sturm's oscillation theorem [13] does not apply for graphs. We shall show however, that Courant's generalization of the oscillation theorem [14] to higher dimensions applies, but much more can be said about the problem. That is, the number of nodal domains of the nth eigenfunction is generically bounded between n and $n_{\min}$ and an explicit expression for $n_{\min}$ will be given.

The rest of this section will be devoted to the introduction of metric graphs and the corresponding Schrödinger operator. The nodal counting problem will be defined in section 2 and some general results will be presented. The distribution of the number of nodal domains will be discussed in section 3. This distribution will be calculated for *star graphs* in section 3.1, and the results of these computations will be used to derive the asymptotic distribution of the number of nodal domains in the limit of large graphs. Some results on counting domains on a bond in star-like graphs will be presented in section 3.1.2. Finally, in section 4 we shall introduce the random wave model for graphs. The mean and variance of the distribution of the number of nodal domains will be computed explicitly and compared with a few numerical results.

A graph $\mathcal{G}$ consist of V *vertices* connected by B *bonds*. The $V \times V$ *connectivity matrix* is defined by

$$C_{i,j} = \text{number of bonds connecting the vertices } i \text{ and } j. \tag{1}$$

A graph is *simple* when for all $i, j : C_{i,j} \in [0, 1]$ (no parallel connections) and $C_{i,i} = 0$ (no loops). The *valence* of a vertex is $v_i = \sum_{j=1}^{V} C_{i,j}$ and the number of bonds is $B = \frac{1}{2}\sum_{i,j=1}^{V} C_{i,j}$. We denote the bond connecting the vertices i and j by $b = [i, j]$. The notation $[i, j]$ and the letter b will be used whenever we refer to a bond without specifying a *direction*: $b = [i, j] = [j, i]$. To any vertex i we can assign the set $S^{(i)}$ of bonds which emanate from it:

$$S^{(i)} = \{\text{all bonds } [i, k] : C_{i,k} = 1\}; \qquad \#[S^{(i)}] = v_i. \tag{2}$$

We assign the natural metric to the bonds. The position x of a point on the graph is determined by specifying on which bond b it is, and its distance x_b from the vertex with the *smaller* index. The length of a bond is denoted by L_b and, $0 \leqslant x_b \leqslant L_b$.

The Schrödinger operator on $\mathcal{G}$ consists of the one-dimensional Laplacian on the bonds, which must be augmented by boundary conditions on the vertices to guarantee that the operator is self-adjoint. We derive the form of the boundary conditions here, since this way we can introduce several of the concepts and definitions to be used later on. Let $x \in \mathcal{G}$ and $\Psi(x)$ be a real valued and continuous function on $\mathcal{G}$, so that $\Psi(x) = \psi_b(x_b)$ for $x \in b$, and $0 \leqslant x_b \leqslant L_b$. The functions $\psi_b(x_b)$ are real valued, bounded with piecewise continuous first derivatives. The set of functions $\Psi(x)$ which fulfil these conditions will be denoted by $\mathcal{D}$ and they are the domain of the (positive definite) quadratic form

$$Q[\Psi] = \int_{\mathcal{G}} \mathrm{d}x \, (\nabla\Psi(x))^2 \equiv \sum_{b=1}^{B} \int_0^{L_b} \mathrm{d}x_b \left(\frac{\mathrm{d}\psi_b}{\mathrm{d}x_b}\right)^2. \tag{3}$$

The unique self-adjoint extension for the Schrödinger operator H, is determined by the Euler–Lagrange extremum principle. The domain of H, $\mathcal{D}_H$ consists of functions in $\mathcal{D}$, with twice differentiable $\psi_b(x_b)$, which satisfy the boundary conditions

$$\forall i = 1, \ldots, V : \sum_{b \in S^{(i)}} n_b(i) \left.\frac{\mathrm{d}\psi_b}{\mathrm{d}x_b}\right|_i = 0, \tag{4}$$

where the derivatives are computed at the common vertex, and $n_b(i)$ takes the value 1 or -1 if the vertex i is approached by taking x_b to 0 or L_b, respectively. These boundary conditions are referred to as the *Neumann* boundary conditions. In the following we shall denote by ϕ_i the value of Ψ at the vertex i.

The spectrum of the Schrödinger operator H is discrete, non-negative and unbounded. It is computed by solving

$$-\frac{\mathrm{d}^2\psi_b^{(n)}(x_b)}{\mathrm{d}x_b^2} = k_n^2 \psi_b^{(n)}(x_b), \qquad \forall b. \tag{5}$$

subject to the boundary conditions (4). The resulting eigenvalues are denoted by k_n^2, and they are ordered so that $k_n \leqslant k_m$ if $n \leqslant m$.

For later use we quote the following property. Let $\mathcal{D}_n$ denote the subspace of functions in $\mathcal{D}$ which are orthogonal to the first $n-1$ eigenfunctions of H. Then, for any non-zero $\Phi \in \mathcal{D}_n$

$$Q[\Phi] \geqslant k_n^2 \int_{\mathcal{G}} \mathrm{d}x (\Phi^2(x)). \tag{6}$$

Equality holds if and only if Φ is the nth eigenfunction of H, $\Psi^{(n)}(x) \in \mathcal{D}_H$ [15].

It is convenient to present the solutions of (5) on the bond $b = [i, j]$ $(i < j)$ as

$$\psi_b(x_b) = \frac{1}{\sin kL_b}(\phi_j \sin kx_b + \phi_i \sin k(L_b - x_b)). \tag{7}$$

The spectrum is computed by substituting (7) into (4), which results in a set of linear and homogeneous equations for the ϕ_i with k dependent coefficients $h_{i,j}(k)$. The spectrum is obtained as the solutions of the equation $\zeta(k) \equiv \det h(k) = 0$. As will be explained shortly, we shall assume that the lengths L_b are *rationally independent*, so that $\zeta(k)$ is an almost periodic function of k. We shall also restrict our attention to simple and connected graphs, and to avoid lengthy discussions of special cases, will assume that the valences $v_i \geqslant 3$ at all the vertices (exceptions will be stated explicitly).

2. Nodal domains on graphs

Nodal domains are connected components of $\mathcal{G}$ where the wavefunction has a constant sign. One cannot exclude the possibility that eigenfunctions of the Schrödinger operator vanish identically on one or several bonds. This is often the case if the bond lengths are rationally dependent. As an example, consider a graph which is composed of two identical sub-graphs which are symmetrically connected by one or several bonds. There exists then an infinite set of wavefunctions which vanish on the connecting bonds. To exclude such cases, we shall discuss graphs with lengths which are *rationally independent (incommensurable)*.

Rational independence is not sufficient to remove completely the possibility that wavefunctions vanish along one or several bonds. To construct an example, take any graph and choose a wavefunction which has a few nodal points on it. Connect the nodal points by bonds and take their length such that the new graph has incommensurate lengths. The Schrödinger operator for the newly constructed graph has the same eigenvalue, and a wavefunction which vanishes identically on all the added bonds. This construction is quite general, but at most, it can bring about a negligible number of such wavefunctions. The reason for this is as follows. If the nth wavefunction on the bond $[i, j]$ vanishes so do both $\phi_i^{(n)}$ and $\phi_j^{(n)}$. The vectors $\phi^{(n)}$ are the null vector of the *quasi-periodic* matrix $h_{i,j}(k_n)$, and as k_n goes over the spectrum, they cover the sphere ergodically. Thus, the probability that several components are exactly 0 is vanishingly small. In what follows we shall ignore this non-generic case and only consider the set of wavefunctions with $\phi_i^{(n)} \neq 0$ for all vertices. Bear in mind, however, that their presence cannot be completely excluded.

The nodal domains on graphs are divided into two types:

(i) *interior domains*—domains which are restricted to single bonds, and whose length is exactly π/k.

(ii) *vertex domains*—domains which include a vertex, and extend to the bonds which emanate from it.

There are V vertex domains, and their length Λ_i can take any value in the range $v_i \frac{\pi}{k} > \Lambda_i \geqslant 0$. Denoting the length of the graph by $\mathcal{L} = \sum_{b=1}^{B} L_b$, we obtain the following expression for the number of nodal domains:

$$\nu_n = V + \frac{k_n}{\pi}\left(\mathcal{L} - \sum_{i=1}^{V} \Lambda_i\right). \tag{8}$$

Note that the second term above is an integer, and that this expression is correct for the generic case where the wavefunction does not vanish along entire bonds. ν_n is bounded in the interval

$$\frac{k_n\mathcal{L}}{\pi} + V \geqslant \nu_n \geqslant \frac{k_n\mathcal{L}}{\pi} + V - 2B. \tag{9}$$

In the limit $n \to \infty$, $\frac{k_n\mathcal{L}}{n\pi} \to 1$. Hence, in this limit, $\frac{\nu_n}{n} \to 1$. This observation stands intermediately between Sturm's oscillation theorem ($\frac{\nu_n}{n} = 1$) and Pleijel's result that $\overline{\lim}\frac{\nu_n}{n}$ is strictly smaller than 1 for the eigenfunctions of the Dirichlet Laplacian for domains in $\mathbb{R}^2$ [15].

An alternative expression for the number of nodal domains provides a sharper bound on the range of variation of ν_n. Denoting the number of *nodal points* on the bond $b = [i, j]$ by $\mu_n^{(b)}$, we have

$$\mu_n^{(b)} = \left[\left[\frac{k_n L_b}{\pi}\right]\right] + \frac{1}{2}\left(1 - (-1)^{[[\frac{k_n L_b}{\pi}]]}\mathrm{sign}[\phi_i]\mathrm{sign}[\phi_j]\right) \tag{10}$$

where $[[x]]$ stands for the largest integer which is smaller than x, and ϕ_i, ϕ_j are the values of the eigenfunction at the vertices i, j respectively. Thus,

$$\nu_n = \sum_{b=1}^{B} \mu_n^{(b)} - B + V. \tag{11}$$

The allowed range for ν_n is now

$$\sum_{b=1}^{B}\left[\left[\frac{k_n L_b}{\pi}\right]\right] + V \geqslant \nu_n \geqslant \sum_{b=1}^{B}\left[\left[\frac{k_n L_b}{\pi}\right]\right] + V - B. \tag{12}$$

The estimates from above can be sharpened by Courant's law [14] adapted for the present problem, which we shall now state and prove.

Theorem. *Let $\mathcal{G}$ be a simple, connected graph. Let k_n^2 be the* nth *eigenvalue of the Schrödinger operator H defined above and let $\Psi_n(x)$ be the corresponding real eigenfunction. Then, the number of nodal domains ν_n of $\Psi_n(x)$ is bounded from above by n, and this bound is optimal.*

The proof follows the method used in [15]. Assume that $\nu_n > n$. Denote by γ_l, the nodal domains on $\mathcal{G}$, so that $\bigcup_{l=1}^{\nu_n} \gamma_l = \mathcal{G}$. Construct n functions $U_l(x) \in \mathcal{D}$ in the following way:

$$U_m(x) = \begin{cases} \Psi_n(x) & \text{if } x \in \gamma_m \\ 0 & \text{otherwise.} \end{cases} \tag{13}$$

It is always possible to find n real constants a_m such that $U(x) = \sum_{m=1}^{n} a_m U_m(x)$ is orthogonal to the first $n - 1$ eigenfunctions of H. Hence $U(x) \in \mathcal{D}_n$. A simple computation shows that

$$Q[U] = k_n^2 \int_{\mathcal{G}} \mathrm{d}x\, U^2(x). \tag{14}$$

However, $U(x)$ is not an eigenfunction, hence the above equality is in contradiction with the strong inequality imposed by (6). Thus, the assumption that $\nu_n > n$ is false. □

In the following sections we shall try to determine how the ν_n values are distributed within their allowed range. We shall start by solving a simpler problem, which pertains to the family of *star graphs*. A similar derivation for more complicated graphs is beyond our present ability. However, assuming that in the limit of large graphs, the lengths of vertex nodal domains are independent, we shall be able to deduce an approximate expression for the distribution of ν_n in this limit.

3. Nodal domain statistics on graphs

In the previous section we observed that $\frac{\nu_n}{n} \to 1$ as $n \to \infty$. Hence, there is no point to use the statistics proposed in [5] for graphs. Rather, we shall discuss the distribution of the quantity

$$\delta\nu_n = \nu_n - n \tag{15}$$

which can vary in the interval $\frac{k_n\pi}{\mathcal{L}} + V - 2B - n \leqslant \delta\nu_n \leqslant 0$. Let $\lambda_n = \frac{k_n}{\pi}\sum_{i=1}^{V}\Lambda_i$ denote the sum of the lengths of the vertex domains measured in units of half the wavelength. Following (8) we find

$$\delta\nu_n = \left[\frac{k_n\mathcal{L}}{\pi} + \frac{1}{2} - n\right] + V - \frac{1}{2} - \lambda_n = \delta N(k_n) + V - \frac{1}{2} - \lambda_n. \tag{16}$$

The expression in square brackets above is the deviation $\delta N(k_n)$ of the mean spectral counting function [12] from its actual value. Thus, the fluctuations in the number of nodal domains stem from two sources: the spectral counting fluctuations, and the fluctuations in the lengths of the *vertex domains* λ_n, whose distribution we shall denote by

$$P(\lambda) = \langle\delta(\lambda - \lambda_n)\rangle, \tag{17}$$

where $\langle\cdots\rangle$ indicates the average over a spectral interval of size Δk, with $\frac{\Delta k\mathcal{L}}{\pi}$ eigenvalues on average. In general, and especially for graphs with small B, the two contributions are probably correlated. For large graphs, however, such correlations are expected to be much weaker. This is the case if the spectral and the eigenvector distributions are independent, like in the relevant random matrix ensemble (GOE). We are not able to prove this statement, and we *assume* that in the limit of large graphs the two contributions can be treated independently. The quantities of interest here are

$$\langle\delta\nu\rangle = \left\langle\left(\frac{k_n\pi}{\mathcal{L}} + \frac{1}{2} - n\right)\right\rangle + V - \frac{1}{2} - \langle\lambda_n\rangle \tag{18}$$

and

$$\langle\Delta\delta\nu^2\rangle \approx \left\langle\Delta\left(\frac{k_n\pi}{\mathcal{L}} + \frac{1}{2} - n\right)^2\right\rangle + \langle\Delta\lambda^2\rangle. \tag{19}$$

The contribution of the spectral fluctuations to the mean $\langle\delta\nu\rangle$, vanishes $\mathcal{O}(\frac{1}{\Delta k})$. λ_n is bounded to $0 \leqslant \lambda_n \leqslant 2B$. In what follows, we shall provide evidence in support of the natural expectation that the λ distribution is symmetric around the point B, thus

$$\langle\lambda\rangle = B. \tag{20}$$

Hence,

$$\langle\nu_n - n\rangle = -(B - V + \tfrac{1}{2}). \tag{21}$$

This result is consistent with $\nu_n - n \leqslant 0$ since we assumed $v_i \geqslant 2$ at all the vertices.

Turning to the variances, the contribution from the spectral counting function for general systems, and for graphs in particular, was studied previously by various authors. We show in the appendix that

$$\langle\delta(N(k_n))^2\rangle = \frac{B}{6}\left(1 + \mathcal{O}\left(\frac{\log B}{B}\right)\right), \tag{22}$$

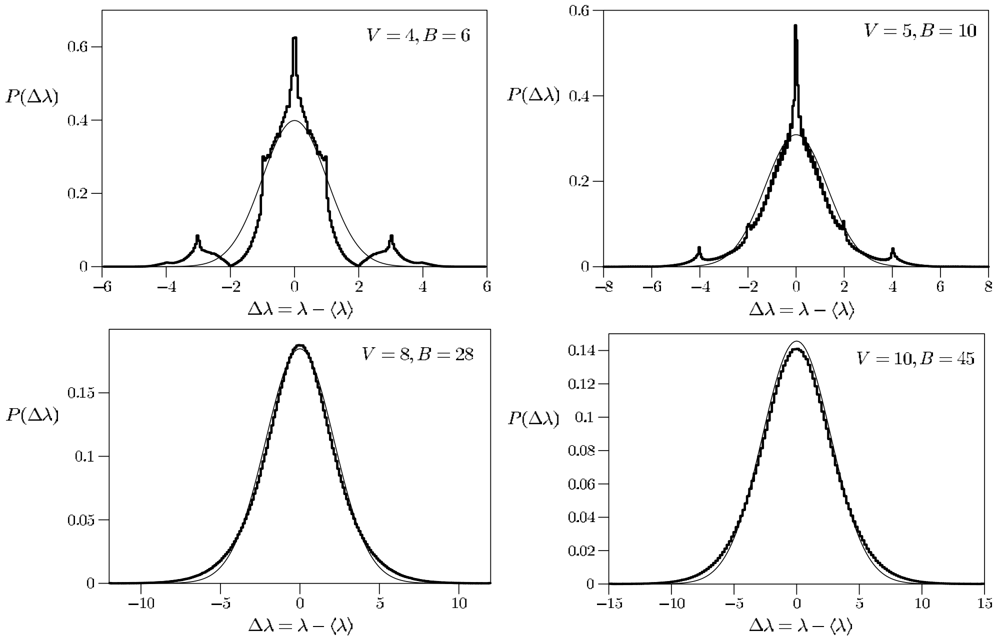

Figure 1. Distribution of the deviation $\Delta\lambda$ of the total length of vertex domains λ from its mean value $\langle\lambda\rangle = B$ for fully connected graphs with $V = 4, 5, 8$ and 10 vertices (in units of half the wavelength). The first 10^7 eigenfunctions have been used for the numerically obtained full curve. The thin curve is a Gaussian of variance $B/6$ where $B = \frac{V(V-1)}{2}$.

The main term in (22) is a universal bound which is valid for all incommensurate Neumann graphs. The error estimate is valid for well connected graphs, where the spectral statistics is known to follow the random matrix predictions. The rest of this and the following sections will deal with the distribution of the total size of the vertex domains λ_n.

The distribution $P(\lambda)$ for a finite small graph shows distinctive features as can be seen in figure 1 where we have plotted the numerically obtained distribution for a fully connected graph with $V = 4$ vertices and $B = 6$ bonds (the *tetrahedron*) and compare it to larger graphs. A bell shaped function is obtained for $P(\lambda)$ of larger graphs which is quite well approximated by a Gaussian of variance $\frac{B}{6}$.

Since λ_n is bounded in the interval $(0, 2B)$ its variance cannot grow faster than B

$$\overline{\Delta\lambda^2} = \beta(\mathcal{G})B, \tag{23}$$

where $\beta(\mathcal{G}) < 1$. We shall compute $\beta(\mathcal{G})$ below for particular models.

A quantity which might be of some interest in the present context is the length (again in units of half the wavelength) $\chi_n^{(i,j)}$ of the intersection of a vertex domain at a given vertex i with the single bond $b = [i, j]$. Generally, $\chi_n^{(i,j)} \neq \chi_n^{(j,i)}$ but they are related by

$$L_{[i,j]} = \frac{\pi}{k_n}\left(\left[\left[\frac{k_n L_{[i,j]}}{\pi}\right]\right] + \chi_n^{(i,j)} + \chi_n^{(j,i)} - \frac{1}{2} - \frac{(-1)^{[[\frac{k_n L_{[i,j]}}{\pi}]]}}{2}\,\mathrm{sign}[\phi_i]\,\mathrm{sign}[\phi_j]\right). \tag{24}$$

The total length of all vertex domains is

$$\lambda_n = \sum_{i<j} C_{i,j}\left(\chi_n^{(i,j)} + \chi_n^{(j,i)}\right). \tag{25}$$

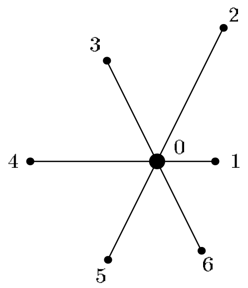

Figure 2. A star graph with $B = 6$ bonds emanating from the central vertex 0.

The distribution

$$P^{(i,j)}(\chi) = \langle \delta(\chi - \chi_n^{(i,j)}) \rangle \tag{26}$$

is thus connected to nodal counting on a single bond. Due to (strong) correlations between the $\chi_n^{(i,j)}$ for different i and j (26) is less useful than (17) or nodal counting on a complete graph.

3.1. Nodal domain statistics on star graphs

In a star graph all bonds emanate star-like from one central vertex $i = 0$. Each bond $b_i = [0, i]$ $(i = 1, \ldots, B)$ connects the central vertex to one *peripheral vertex i* (see figure 2). The bond b_i has length L_i and all lengths are chosen incommensurate. The variable x_i measures the distance from the centre on bond b_i such that $0 \leqslant x_i \leqslant L_i$ and $x_i = L_i$ at the peripheral vertex i. Though the number of vertices is $V = B + 1$ only the central vertex fulfils $v_0 \geqslant 3$ (if $B \geqslant 3$). The peripheral vertices have valence $v_i = 1$ and instead of Neumann boundary conditions we will use Dirichlet boundary conditions $\phi_i = 0$ $(i = 1, \ldots, B)$ there. The wavefunction on the bond b_i follows from (7)

$$\psi_i(x_i) = \frac{\phi_0}{\sin kL_i} \sin k(L_i - x_i) \tag{27}$$

where ϕ_0 is the value of the wavefunction on the central vertex. Current conservation at the centre leads to the quantization condition

$$f_B(k_n) \equiv \sum_{i=1}^{B} \cot k_n L_i = 0 \tag{28}$$

for the nth eigenvalue k_n of the star graph [16].

Since the peripheral vertices are nodal points, equations (8) and (16) for the number of nodal domains have to be modified to

$$\nu_n = 1 + \sum_{i=1}^{B} \left[\!\left[\frac{L_i k_n}{\pi} \right]\!\right] = 1 + \frac{k_n}{\pi}\mathcal{L} - \lambda_n \tag{29}$$

where $\lambda_n = \frac{k_n \mathcal{L}}{\pi} - \sum_{i=1}^{B} [\![\frac{L_i k_n}{\pi}]\!]$ is $\frac{k_n}{\pi}$ times the length of the nodal domain that contains the central vertex. Obviously $0 \leqslant \lambda_n \leqslant B$ and ν_n is bounded by

$$1 + \frac{k_n \mathcal{L}}{\pi} \geqslant \nu_n \geqslant 1 - B + \frac{k_n \mathcal{L}}{\pi}. \tag{30}$$

3.1.1. The central nodal domains. As discussed above, nodal counting is partly determined by spectral fluctuations and partly by the distribution (17) of the length λ of the central nodal domain. We shall consider here only the distribution of the lengths of the central vertex domain,

$$P(\lambda) = \langle \delta(\lambda - \lambda_n) \rangle = \lim_{\Delta k \to \infty} \frac{\pi}{\Delta k \mathcal{L}} \int_0^{\Delta k} \mathrm{d}k \left| \frac{\mathrm{d} f_B}{\mathrm{d}k}(k) \right| \delta(f_B(k)) \delta(\lambda - \lambda(k)) \tag{31}$$

where $\lambda(k) = \sum_{i=1}^{B} (\frac{kL_i}{\pi} - [\![\frac{kL_i}{\pi}]\!])$. From (28) we have

$$\frac{\mathrm{d} f_B}{\mathrm{d}k}(k) = -\sum_{i=1}^{B} \frac{L_i}{\sin^2 kL_i} \leqslant 0. \tag{32}$$

Let

$$\chi_i = \frac{kL_i}{\pi} - \left[\!\left[\frac{kL_i}{\pi} \right]\!\right] \tag{33}$$

be the (rescaled) length of the intersection of the central nodal domain with the ith bond ($\lambda(k) = \sum_{i=1}^{B} \chi_i$). Obviously, $0 \leqslant \chi_i \leqslant 1$ and since the length L_i are assumed incommensurate, k creates an ergodic flow on the B-torus spanned by the χ_i [17]. Thus, the spectral integral over k in (31) may be replaced by an integral over the B-torus variables χ_i. This leads to

$$P(\lambda) = \pi \int_0^1 \mathrm{d}^B \chi \, \frac{1}{\sin^2 \pi \chi_1} \, \delta\left(\sum_{i=1}^{B} \cot \pi \chi_i \right) \delta\left(\lambda - \sum_{i=1}^{B} \chi_i \right). \tag{34}$$

Replacing the two δ-functions by their Fourier representation, the distribution takes the form

$$P(\lambda) = \frac{1}{4\pi} \int_{-\infty}^{\infty} \mathrm{d}\eta \int_{-\infty}^{\infty} \mathrm{d}\xi \, G(\eta, \xi)^{B-1} \tilde{G}(\eta, \xi) \, \mathrm{e}^{\mathrm{i}\xi(\lambda - \frac{B}{2})} \tag{35}$$

where

$$G(\eta, \xi) = \frac{2}{\pi} \int_0^{\frac{\pi}{2}} \mathrm{d}\alpha \, \cos\left(\eta \tan \alpha + \frac{\xi}{\pi} \alpha \right) \tag{36}$$

and

$$\tilde{G}(\eta, \xi) = \left(1 - \frac{\partial^2}{\partial \eta^2} \right) G(\eta, \xi) = 2 \cos \frac{\xi}{2} \delta(\eta) - \frac{\xi}{\pi} G(\eta, \xi) \mathbb{P} \frac{1}{\eta}. \tag{37}$$

The last line shows that $\tilde{G}(\eta, \xi)$ is a distribution where $\mathbb{P}\frac{1}{\eta}$ denotes Cauchy's principal value. The integral (36) can be solved explicitly (see [18], (3.718)) in terms of Whittaker functions $W_{\mu,\nu}(x)$

$$G(\eta, \xi) = \Theta(\eta) \frac{W_{-\frac{\xi}{2\pi}, \frac{1}{2}}(2\eta)}{\Gamma(1 - \frac{\xi}{2\pi})} + \Theta(-\eta) \frac{W_{\frac{\xi}{2\pi}, \frac{1}{2}}(-2\eta)}{\Gamma(1 + \frac{\xi}{2\pi})}. \tag{38}$$

Here $\Theta(x)$ is Heaviside's step function. The appearance of Whittaker functions can also be seen from (37)—for $\eta \neq 0$ the right-hand sides reduce to $(1 - \frac{\partial^2}{\partial \eta^2}) G(\eta, \xi) = -\frac{\xi}{\pi \eta} G(\eta, \xi)$, a special case of Whittaker's differential equation [18]. Using the last line of equation (37) the distribution can be written as a sum of two terms $P(\lambda) = P_\delta(\lambda) + P_{\mathbb{P}}(\lambda)$ where

$$P_\delta(\lambda) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}\xi \int_{-\infty}^{\infty} \mathrm{d}\eta\, G(\eta,\xi)^{B-1}\,\delta(\eta)\cos\frac{\xi}{2}\cos\left(\xi\left(\lambda-\frac{B}{2}\right)\right)$$
$$= \frac{2}{\pi}\int_0^\infty \mathrm{d}z\left(\frac{\sin z}{z}\right)^{B-1}\cos z\cos(z(2\lambda-B))$$
$$= \frac{B-1}{2}\sum_{0\leqslant l<\frac{B}{2}}\frac{(-1)^l}{l!(B-1-l)!}\left(\Theta\left(\frac{B}{2}-l-\left|\lambda-\frac{B}{2}\right|\right)\left(\frac{B}{2}-l-\left|\lambda-\frac{B}{2}\right|\right)^{B-2}\right.$$
$$\left.+\,\Theta\left(\frac{B}{2}-1-l-\left|\lambda-\frac{B}{2}\right|\right)\left(\frac{B}{2}-1-l-\left|\lambda-\frac{B}{2}\right|\right)^{B-2}\right) \tag{39}$$

and

$$P_{\mathbb{P}}(\lambda) = -\frac{1}{4\pi^2}\int_{-\infty}^{\infty}\mathrm{d}\xi\,\xi\cos\left(\xi\left(\lambda-\frac{B}{2}\right)\right)\int_{-\infty}^{\infty}\mathrm{d}\eta\,\mathbb{P}\frac{1}{\eta}G(\eta,\xi)^B$$
$$= \frac{2}{\pi^2}\int_0^\infty \mathrm{d}z\, z\cos(z(2\lambda-B))$$
$$\times\int_0^\infty \mathrm{d}y\,\frac{1}{y}\left(\left(\frac{W_{\frac{z}{\pi},\frac{1}{2}}(y)}{\Gamma\left(1+\frac{z}{\pi}\right)}\right)^B-\left(\frac{W_{-\frac{z}{\pi},\frac{1}{2}}(y)}{\Gamma\left(1-\frac{z}{\pi}\right)}\right)^B\right). \tag{40}$$

$P(\lambda)$ is symmetric in $\lambda-\frac{B}{2}$. Hence $\langle\lambda\rangle = \frac{B}{2}$.

For large star graphs ($B \gg 1$), $P(\lambda)$ is dominated by $P_\delta(\lambda)$ (see figure 3). This observation is supported by the fact that $P_{\mathbb{P}}(\lambda)$ does not contribute to the integrated probability distribution, $\int_{-\infty}^{\infty}\mathrm{d}\lambda\, P_{\mathbb{P}}(\lambda) = 0$ while $\int_{-\infty}^{\infty}\mathrm{d}\lambda\, P_\delta(\lambda) = 1$. The dominance of $P_\delta(\lambda)$ can be further supported by computing the variance of the exact distribution $P(\lambda)$ and of $P_\delta(\lambda)$. The exact variance is evaluated by going back to (34):

$$\langle\Delta\lambda^2\rangle = \int \mathrm{d}\lambda\left(\lambda-\frac{B}{2}\right)^2 P(\lambda)$$
$$= \pi\int_0^1 \mathrm{d}^B\chi\,\frac{1}{\sin^2\pi\chi_1}\,\delta\left(\sum_{i=1}^B\cot\pi\chi_i\right)\left(\frac{B}{2}-\sum_{i=1}^B\chi_i\right)^2$$
$$= \frac{B+2}{12}-\frac{4}{\pi}\int_0^{\frac{1}{2}}\mathrm{d}z\, z\arctan\frac{\tan z\pi}{B-1}$$
$$= \frac{B+2}{12}+\mathcal{O}(B^{-1-\rho}), \qquad (\rho>0). \tag{41}$$

Using (39) we reproduce the leading terms in the exact variance:

$$\int \mathrm{d}\lambda\left(\lambda-\frac{B}{2}\right)^2 P_\delta(\lambda) = \frac{B+2}{12}. \tag{42}$$

The fact that $P_\delta(\lambda)$ approaches $P(\lambda)$ for large star graphs is very important in the present context. First, it provides an analytic expression, which for large B tends to a Gaussian with a variance given by (42). Second, when we consider general large graphs, the size of the vertex domains become statistically independent, and their distribution can be approximated by a Gaussian whose variance is

$$\langle(\Delta\lambda)^2\rangle \approx \frac{1}{12}\sum v_i = \frac{B}{6}, \tag{43}$$

where now B stands for the number of bonds on the general graph.

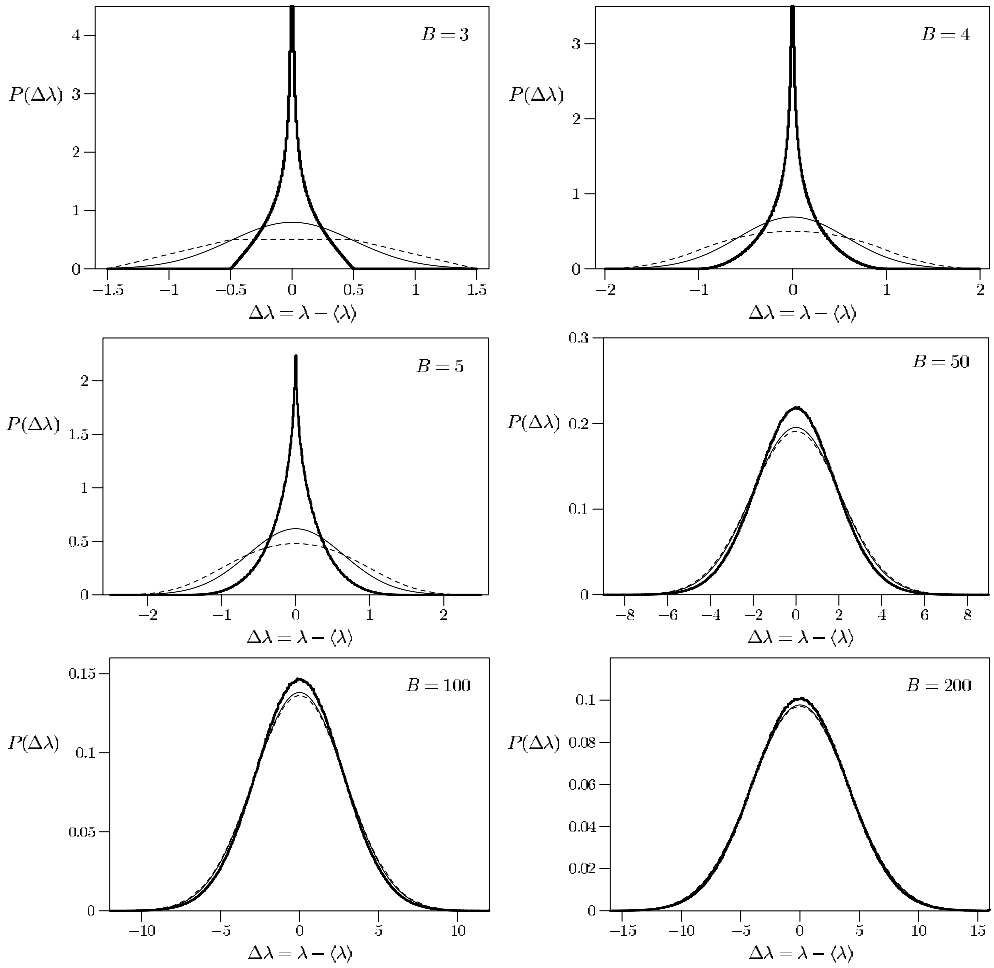

Figure 3. Numerically obtained distributions of the length of the central nodal domain in a star graph with $B = 3$, 4, 5, 50, 100 and 200 bonds (histograms—full curves)—the first 2×10^6 eigenfunctions have been used for each graph. The dashed curve gives $P_\delta(\lambda) = P(\lambda) - P_{\mathbb{P}}(\lambda)$ and the thin curve is a Gaussian with variance $\frac{B}{12}$—for large B the Gaussian is indistinguishable from $P_\delta(\lambda)$ and the numerical distribution slowly converges to the Gaussian.

Combining the two estimates for the variances of the spectral fluctuations (22) and the nodal domain fluctuations (43), we obtain the leading term for the variance of the number of nodal domains:

$$\langle(\Delta\nu)^2\rangle = \frac{B}{3}. \tag{44}$$

This estimate holds in the limit of large graphs. In the next section we shall show that the random wave model for the graph provides the same answer for the variance (and the mean) of the nodal domain distribution.

3.1.2. Nodal domains on a single bond. In a star graph the number of nodal domains on the bond $b_i = [0, i]$ is

$$\left[\left[\frac{k_n L_i}{\pi}\right]\right] = \frac{k_n L_i}{\pi} - \chi_i \tag{45}$$

where χ_i is the length of the intersection of the central nodal domain with the bond b_i as in equation (33) above. Note, that there are no vertex domains on the peripheral vertices and equation (24) has to be modified. Following the preceding section we define

$$
\begin{aligned}
P^{(i)}(\chi) &= \lim_{\Delta k\to\infty} \frac{\pi}{\Delta k \mathcal{L}} \int_0^{\Delta k} \mathrm{d}k \left| \frac{\mathrm{d} f_B}{\mathrm{d}k}(k) \right| \delta(f_B(k)) \delta(\chi - \chi_i(k)) \\
&= \pi \int_0^1 \mathrm{d}^B \chi \, \delta\left(\sum_{i=1}^{B} \cot \pi \chi_i \right) \delta(\chi - \chi_i) \sum_{j=1}^{B} \frac{L_j}{\mathcal{L} \sin^2 \pi \chi_j}. \qquad (46)
\end{aligned}
$$

With similar techniques as in the previous section this integral can be solved explicitly:

$$
P^{(i)}(\chi) = \frac{\mathcal{L} - L_i}{\mathcal{L}} + \frac{L_i}{\mathcal{L}} \frac{B-1}{(B-1)^2 \sin^2 \chi\pi + \cos^2 \chi\pi}. \qquad (47)
$$

For large star graphs $B \gg 1$ where each bond length is of similar size one has $\frac{L_i}{\mathcal{L}} \sim \frac{1}{B}$ and the distribution becomes uniform (with two singular points at $\chi = 0$ and 1). If one bond length L_i exceeds the other bond lengths such that $L_i \gg \mathcal{L} - L_i$ the distribution becomes

$$
P^{(i)}(\chi) \approx \frac{B-1}{(B-1)^2 \sin^2 \chi\pi + \cos^2 \chi\pi} \qquad (48)
$$

which for large B is peaked at $\chi = 0$ and π.

4. Random waves on graphs

Since Berry's seminal work [11] random waves have been a paradigm for chaotic wavefunctions. Recently they have been used extensively in the investigation of the nodal structure in chaotic wavefunctions [5–10].

In this section we will introduce random waves on graphs. Any ensemble of random waves should solve Schrödinger's equation on the bonds and be continuous at the vertices. Thus, any set of values $\{\phi_j\}$ $(j = 1, \ldots, V)$ for the wavefunction on the vertices determines a wavefunction on the graph which solves (7). However, these waves do not fulfil the correct boundary conditions (current conservation) on the graph. The ensemble of random waves on a graph is therefore defined in terms of the probability distribution of ϕ_j.

Before we define the appropriate ensemble for more general graphs it will be instructive to discuss star graphs. If we want to compare random waves with the star graph results of the previous chapter we have to keep the Dirichlet boundary conditions at the peripheral vertices and only relax the current conservation condition at the centre. Then $\psi_i(x_i) = \frac{\phi_0}{\sin k L_i} \sin k(L_i - x_i)$ is the random wave on the ith bond and ϕ_0 is the only random parameter for fixed k. Obviously the position of nodal points does not depend on ϕ_0. Thus, we do not need the distribution $P(\phi_0)$ for the discussion of nodal domain statistics. Let us now rewrite equation (29) for the number of nodal domains

$$
\begin{aligned}
\nu(k) &= 1 + \sum_{i=1}^{B} \int_{1/2}^{L_i} \mathrm{d}x_i \sum_{j=-\infty}^{\infty} \delta(x_i - j) \\
&= 1 + \frac{k\mathcal{L}}{\pi} - \frac{B}{2} + \sum_{i=1}^{B} \sum_{j=1}^{\infty} \frac{\sin 2\pi j L_i k}{j\pi}. \qquad (49)
\end{aligned}
$$

Averaging over a k-interval reveals that the mean is $\bar{\nu} = 1 + \frac{k\mathcal{L}}{\pi} - \frac{B}{2}$ which coincides with the result for the eigenfunctions in the previous chapter. For the variance we get

$$
\overline{\Delta\nu^2} = \int_{k_0}^{k_0+\Delta k} \sum_{i,i'=1}^{B} \sum_{j,j'=1}^{\infty} \frac{\cos 2\pi k(jL_i - j'L_{i'}) - \cos 2\pi k(jL_i + j'L_{i'})}{2\Delta k j j' \pi^2}
$$

$$= \frac{B}{2\pi^2}\sum_{j=1}^{\infty}\frac{1}{j^2} + \mathcal{O}(\Delta k^{-1}) = \frac{B}{12} + \mathcal{O}(\Delta k^{-1}) \tag{50}$$

which again coincides with the result for the eigenfunctions of star graphs for large B. Note, that for incommensurate bond lengths there are no correlations between the contributions from single bonds. Thus the number of nodal domains is a sum of independent quantities each of finite variance. The central limit theorem leads to Gaussian statistics for large B.

To define an appropriate ensemble for more general graphs we will be guided by wavefunctions that *do* fulfil current conservation (we will again assume that each vertex has a valence $v_i \leqslant 3$). The quantization condition for a graph has the form $\det h_{ij}(k) = 0$ where $h_{ij}(k)$ is a real symmetric matrix of dimension $V \times V$ [12]. If the quantization condition is fulfilled for k, the eigenvector for the zero eigenvalue is a set of vertex values $\{\phi_j\}$ that determines the eigenfunction. For incommensurate lengths $h_{ij}(k)$ is a quasi-periodic function of k such that the matrices $h_{ij}(k)$ are expected to be typical members of the Gaussian orthogonal ensemble (GOE) in random-matrix theory. Since for that ensemble eigenvectors have uncorrelated components, we will *assume* for the ensemble of random waves on the graph that ϕ_j are independent Gaussian variables of equal variance. From equations (10) and (11) we see that the number of nodal domains only depends on the signs of ϕ_j. Let $\sigma_j = \text{sign}[\phi_j]$, then $\sigma_j = \pm 1$ with equal probability. The number of nodal domains can now be rewritten as

$$\nu(k) = \frac{k\mathcal{L}}{\pi} + V - B + \sum_{i,j:i<j} C_{i,j}\left(\sum_{m=1}^{\infty}\frac{\sin 2\pi mkL_{ij}}{m\pi} - \frac{1}{2}(-1)^{[[\frac{kL_{ij}}{\pi}]]}\sigma_i\sigma_j\right). \tag{51}$$

Averaging over a k-interval of length Δk centred at k_0 and over σ_j gives the mean number of nodal domains

$$\langle\nu\rangle = \frac{k_0\mathcal{L}}{\pi} + V - B + \mathcal{O}(\Delta k^{-1}). \tag{52}$$

The variance of the number of nodal domains is purely due to the sum over i, j in (51). To leading order, the sum over sines and the sum over the signs σ_i give independent contributions to the variance. We have already calculated the first part $\langle\nu^2\rangle_{\sin} = \frac{B}{12}$ above in our discussion of random waves on star graphs. The fluctuations due to the signs are stronger, and they provide to the variance a term $\overline{\nu^2}_\sigma = \frac{B}{4}$. Hence the random wave model predicts the variance

$$\overline{\nu^2} = \frac{B}{3} + \mathcal{O}(\Delta k^{-1}). \tag{53}$$

This result reproduces the estimate (44), which was derived under very different assumptions. Finally we would like to note that bonds do not contribute independently to the number of nodal domains. However, these correlations are not expressed in the variance. They do contribute, however to the higher moments.

The random wave models enable us in principle to write down an explicit formula for the probability density of the number of nodal domains.

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Appendix

In this appendix we justify the bound (22) on the variance of the spectral counting function for graphs.

The starting point is the expression of the spectral counting function $N(k)$ as a sum of its mean value (Weyl's law) and an oscillatory part,

$$N(k) = \frac{k\mathcal{L}}{\pi} + \frac{1}{2} + \delta N(k), \tag{54}$$

and the oscillatory part is given by [12]

$$\delta N(k) = \frac{1}{\pi} \operatorname{Im} \sum_{m=1}^{\infty} \frac{\operatorname{tr}(\mathcal{S}_{\mathrm{B}}(k))^m}{m}. \tag{55}$$

$\mathcal{S}_{\mathrm{B}}(k_n)$ is the *bond scattering matrix* defined in [12]. $\operatorname{tr}(\mathcal{S}_{\mathrm{B}}(k))^m$, is a sum of contributions from all the m-periodic orbits on the graph. Each contribution is endowed with a phase proportional to kl_p^m, where l_p^m is the length of the orbit, and p is the summation index. Because of the rational independence of the bond lengths,

$$\langle \operatorname{tr}(\mathcal{S}_{\mathrm{B}}(k))^m \operatorname{tr}(\mathcal{S}_{\mathrm{B}}^*(k))^n \rangle = 2BK_m\delta_{m,n} + \mathcal{O}(\Delta k^{-1}) \tag{56}$$

where K_m is the spectral form factor associated with the graph [19]. The mere fact that the bond lengths of the graph are not commensurate, is enough to guarantee that on average $K_m \leqslant 1$:

$$\langle (\delta N(k))^2 \rangle \approx \frac{1}{2\pi^2} \sum_{m=1}^{\infty} \frac{\langle | \operatorname{tr}(\mathcal{S}_{\mathrm{B}}(k))^m|^2 \rangle}{m^2} \leqslant \frac{B}{6}. \tag{57}$$

A sharper estimate can be given for well connected graphs, where numerical and analytic results [12, 20] show that K_m follow the predictions of random matrix theory for the circular orthogonal ensemble (COE). We can use the known functional dependence of K_m on m and B [21] and show that

$$\langle (\delta N(k))^2 \rangle = \frac{B}{6}\left(1 + \mathcal{O}\frac{\log B}{B}\right). \tag{58}$$

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