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Anomalous nodal count and singularities in the dispersion relation of honeycomb graphs

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We study the nodal count of the so-called bi-dendral graphs and show that it exhibits an anomaly: the nodal surplus is never equal to 0 or β, the first Betti number of the graph. According to the nodal-magnetic theorem, this means that bands of the magnetic spectrum (dispersion relation) of such graphs do not have maxima or minima at the "usual" symmetry points of the fundamental domain of the reciprocal space of magnetic parameters. In search of the missing extrema, we prove a necessary condition for a smooth critical point to happen inside the reciprocal fundamental domain. Using this condition, we identify the extrema as the singularities in the dispersion relation of the maximal Abelian cover of the graph (the honeycomb graph being an important example). In particular, our results show that the anomalous nodal count is an indication of the presence of conical points in the dispersion relation of the maximal universal cover. We also discover that the conical points are present in the dispersion relation of graphs with much less symmetry than was required in previous investigations. © *2015 AIP Publishing LLC.* [http://dx.doi.org/10.1063/1.4937119]

I. INTRODUCTION

Quantum graphs and discrete graphs play a significant role in numerous recent investigations in mathematical physics. On one side, their importance is apparent in the fields of quantum chaos and spectral theory.[35,29,38,11] On the other side, they are applied to model various quasi one-dimensional physical systems such as photonic networks, nanostructures, and waveguides.[37,11,44] The current work exposes a curious link between what has so far been considered a more theoretical aspect of spectral theory on graphs, the nodal count of eigenfunctions, and a phenomenon with wide-ranging applied consequences, the existence of Dirac points in the dispersion relation of periodic structures.

The study of zeros of a quantum graph's eigenfunctions is a fertile area of research with many questions which are still open. Some recent results include bounds on the number of nodal domains,[43,30,46,7] specific formulae for some classes of graphs,[5] variational characterizations,[4,13] and inverse problems.[2] To highlight just one key result, it was proven in a sequence of works by different authors (see Refs. 7 and 4 and references within) that the number ϕ_n of zeros of the nth eigenfunction obeys the bounds,

$$0 \leq \phi_n - (n-1) \leq \beta,$$

where β is the first Betti number of the graph (intuitively, the number of cycles). A natural next question is to consider the distribution of the values $\{\phi_n - (n-1)\}_{n=1}^{\infty}$. One would expect, for example, from the magnetic variational characterization of the "nodal surplus" $\phi_n - (n-1)$,[8,13] that all the integers between 0 and β appear infinitely often as the nodal surplus of any graph with Betti number β. However, in the current work, we show that there is a family of graphs for which this distribution is not supported on the lower and upper bounds (0 and β). Those are the graphs which are obtained as two copies of a tree graph glued together at their corresponding leaves. Hence, they are called bi-dendral graphs (see Figure 1(a) for an example). When the underlying tree is actually a star graph (i.e., a graph with one central vertex connected to all other vertices which are degree

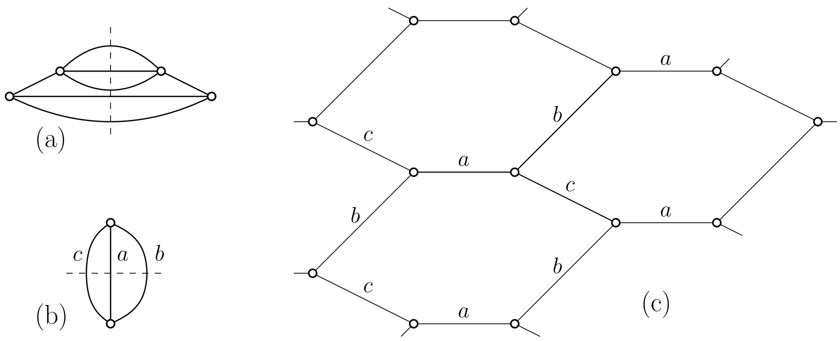

FIG. 1. An example of a bi-dendral graph (a), the symmetry axis is indicated by the dashed line; a 3-mandarin graph (b) and its maximal Abelian cover (c). The Abelian cover graph has honeycomb structure although less symmetry than a regular honeycomb lattice: only the parallel edges have the same length.

one), we call the resulting bi-dendral graph a mandarin graph. We prove that the above nodal count anomaly implies the presence of special singularities in the dispersion relation of the Abelian cover version of the mandarin graph. This Abelian cover is a periodic infinite graph, also known as the honeycomb graph; it is a tiling of the plane by congruent hexagons whose parallel edges are of equal length (Figure 1(c)).

Periodic infinite quantum graphs have been fruitfully used to model diverse physical systems such as photonic crystals,[39] graphene,[40] and its allotropes.[20] The Floquet-Bloch theory (see chapter 4 in Ref. 11) reduces the problem of determining the continuous spectrum of a periodic graph to the study of a parameter-dependent operator on a compact graph. The parameters can be interpreted as magnetic fluxes through the graph; the (now discrete) spectrum as a function of these parameters is called the dispersion relation. The points where two sheets of the dispersion relation touch are of particular interest, as many physical properties of the material are related to the location of these points (so-called Dirac points) and the structure of the bands in their vicinity.[15,42,22,33,23] The current work characterizes the location of the Dirac points and the structure of the corresponding eigenstates for periodic graphs, which are the Abelian covers of the mandarin graphs. This is particularly important as one member of this family (the 3-mandarin) is exactly the well-studied hexagonal lattice which models graphene, although with much reduced symmetry. The presence of the Dirac points is the explanation for the anomaly in the nodal count (see Section III); conversely, the anomalous count is an indication of existence of singularities in the dispersion relation. The connection between the two is provided by the "magnetic-nodal" theorem.[8,17,13]

Section II introduces Schrödinger operators on quantum graphs and Section III presents the main results of the paper. Section IV contains the proof of the anomaly of the bi-dendral graph nodal count, to which we arrive by establishing new eigenvalue interlacing results. Section V studies the dispersion relation of general periodic graphs and then discusses the Abelian cover of the mandarin graph and makes the connection with its nodal count. Finally, in the Appendix, we adapt the results of Section V to discrete graphs.

II. SCHRÖDINGER OPERATORS ON QUANTUM GRAPHS

We start by defining a quantum graph, following the notational conventions of Ref. 11, which also contains the proofs of the background results used in this section.

Let Γ be a compact metric graph with vertex set V and edge set E. Let $\widetilde{H}^k(\Gamma,\mathbb{C})$ be the space of all complex-valued functions that are in the Sobolev space $H^k(e)$ for each edge, or in other words

$$\widetilde{H}^k(\Gamma,\mathbb{C}) = \bigoplus_{e\in E} H^k(e).$$

Consider the Schrödinger operator with electric potential $q : \Gamma \to \mathbb{R}$ defined by

$$H^0 : f \mapsto -\frac{d^2 f}{dx^2} + qf,$$

acting on the functions from $\widetilde{H}^2(\Gamma,\mathbb{C})$ satisfying the δ-type matching conditions

$$\begin{cases} f(x) \text{ is continuous at } v, \\ \displaystyle\sum_{e\in E_v} \frac{df}{dx_e}(v) = \chi_v f(v), \qquad \chi_v \in \mathbb{R} \end{cases} \tag{2.1}$$

at all vertices $v \in V$. Here, the potential $q(x)$ is assumed to be piecewise continuous. The set E_v is the set of edges joined at the vertex v; by convention, each derivative at a vertex is taken into the corresponding edge. We denote by x_e the local coordinate on the edge e. On vertices of degree more than one we usually take $\chi_v = 0$, the so-called Neumann condition. Non-zero χ_v will be used on vertices of degree one, where we also allow the Dirichlet condition $f(v) = 0$, which is formally equivalent to $\chi_v = \infty$. We note that a Neumann vertex of degree two can be absorbed into its neighboring edges unifying them both to a single edge (whose length equals the sum of both), without changing the graph spectral properties. At vertices of degree two, we will sometimes be using the so-called anti-Neumann vertex condition. Namely, for a vertex v of degree two, which is connected to the edges e_+ and e_-, the anti-Neumann condition is

$$f|_{e_-}(v) = -f|_{e_+}(v), \qquad f'|_{e_-}(v) = f'|_{e_+}(v), \tag{2.2}$$

where the direction of the derivative is taken from the vertex v into the edge $e_\pm$. Note that the anti-Neumann condition does not fall in the class of vertex conditions (2.1).

The operator H^0 is self-adjoint, bounded from below, and has a discrete set of eigenvalues that can be ordered as

$$\lambda_1 \le \lambda_2 \le \cdots \le \lambda_n \le \cdots.$$

Throughout the paper, we will frequently assume that the graph's eigenvalues and eigenfunctions are generic in the following sense.

Definition 2.1.

(1) The eigenpair (λ, f) is called generic if the eigenvalue λ is simple and the corresponding eigenfunction f is different than zero on every vertex.
(2) Both λ and f in a generic pair are also called generic.
(3) A quantum graph is generic if all of its eigenpairs are generic.

The conditions which guarantee the graph's genericity are discussed in Refs. 28 and 12. We will count zeros only for generic eigenfunctions.

Definition 2.2.

(1) Let f_n be a generic eigenfunction corresponding to the nth eigenvalue, λ_n (counting with multiplicities). Denote by ϕ_n, the number of its internal zeros. Namely, we do not include the Dirichlet vertices, if they exist, in the count.
(2) The quantity $\sigma_n := \phi_n - (n-1)$ is called the nodal surplus.

It was recently discovered that the graph's nodal count is closely related to properties of the magnetic Schrödinger operator on the graph. This connection is described in Theorem 2.3. The magnetic Schrödinger operator on Γ is given by

$$H^A(\Gamma) : f \mapsto -\left(\frac{d}{dx} - iA(x)\right)^2 f + qf, \qquad f \in \widetilde{H}^2(\Gamma,\mathbb{C}),$$

where the magnetic potential, $A(x)$, is a one-form (namely, the sign of $A(x)$ changes with the orientation of the edge). The δ-type boundary conditions are now modified to the following at all vertices $v \in V$:

$$\begin{cases} f(x) \text{ is continuous at } v, \\ \displaystyle\sum_{e\in E_v} \left(\frac{df}{dx_e}(v) - iA(v)f(v)\right) = \chi_v f(v), \qquad \chi_v \in \mathbb{R}. \end{cases}$$

Let $\beta = |E| - |V| + 1$ be the first Betti number of the graph Γ, i.e., the rank of the graph's fundamental group. Informally speaking, β is the number of "independent" cycles on the graph and hence is zero if the graph is a tree. Up to a change of gauge, a magnetic field on a graph is fully specified by β fluxes $\alpha_1, \alpha_2, \ldots, \alpha_\beta$, defined as

$$\alpha_j = \oint_{\tau_j} A(x)dx \mod 2\pi,$$

where $\{\tau_j\}$ is a set of generators of the fundamental group. In other words, magnetic Schrödinger operators with different magnetic potentials $A(x)$, but the same fluxes $(\alpha_1, \ldots, \alpha_\beta)$, are unitarily equivalent. Therefore, the eigenvalues $\lambda_n(H^A)$ can be viewed as functions of $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_\beta)$. The connection between this function and the nodal count is explicated in the following theorem.

Theorem 2.3. *Let (λ_n, f_n) be a generic eigenpair of H^A with A corresponding to some flux $\boldsymbol{\alpha}^* \in \{0, \pi\}^\beta$. Then, $\boldsymbol{\alpha}^*$ is a non-degenerate critical point of the function $\lambda_n(\boldsymbol{\alpha})$ and its Morse index is equal to the nodal surplus, σ_n.*

Remark 2.4. The above theorem is proved in Ref. 13 for $\boldsymbol{\alpha} = (0, \ldots, 0)$, extending to quantum graphs an earlier result on discrete graphs[8] (also see Ref. 17). One may repeat the same proof from Ref. 13 for all other $\boldsymbol{\alpha} \in \{0, \pi\}^\beta$, noticing the following:

(1) Introducing a vertex of degree two with an anti-Neumann vertex condition on some edge results in an operator which is unitarily equivalent to the original operator with a magnetic potential on this edge integrating to π.
(2) The anti-Neumann condition keeps the operator self-adjoint and does not change either of the quadratic forms used in section 4 of Ref. 13; the only change needed is the additional condition $f\big|_{e_-}(v) = -f\big|_{e_+}(v)$ imposed on the domain of the quadratic form.
(3) The nth eigenfunction of a tree graph has $n-1$ internal zeros and this holds even if some anti-Neumann conditions are imposed on the graph (relevant for the proof of Theorem 3.3, part 1 in Ref. 13).

As a corollary, we get an earlier result (see Refs. 7 and 4 and references therein),

$$0 \le \sigma_n \le \beta. \tag{2.3}$$

The theorem above makes one wonder whether the whole range of integers from 0 to β is covered by σ_n for any graph. We will show that there is a family of quantum graphs for which the answer to this question is negative. These graphs, to be discussed next, and their spectral properties are the focus of this paper.

III. MAIN RESULTS

A. Anomalous nodal count

Consider two copies of a tree graph with d leaves (vertices of degree one) which are glued together by identifying corresponding leaves of both. We impose Neumann conditions at all vertices and call the resulting quantum graph a *bi-dendral graph*. When the underlying tree graph is chosen to be a star graph, we obtain a graph consisting of two vertices and d edges connecting them (recalling that Neumann vertices of degree two can be absorbed into an edge). We will call such a graph a *d-mandarin graph* (see Figure 1). A bi-dendral graph has an obvious symmetry axis which passes through all points arising from gluing the leaves. We call the edges which cross this symmetry axis the *middle edges*. We extend the definition of a bi-dendral graph by allowing for vertices of degree two with anti-Neumann condition to be present on those middle edges. Finally, we will be assuming the graph edge lengths are chosen such that either a particular eigenvalue is generic or the graph is generic (see Definition 2.1).

Theorem 3.1. *Let Γ be a bi-dendral graph with d middle edges, such that $a \ge 0$ of them have anti-Neumann conditions imposed at an intermediate point. If the nth eigenpair is generic and*

$n > 1$ or $a > 0$, then the nodal surplus σ_n satisfies

$$1 \le \sigma_n \le \beta - 1 = d - 2. \tag{3.1}$$

Remark 3.2. Compare (3.1) with the general bounds of the nodal surplus, (2.3).

Consider the eigenvalue $\lambda_n(\boldsymbol{\alpha})$ as a function of $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_\beta)$, the total fluxes through the cycles of the graph (for some pre-fixed basis of the fundamental group). It is well-known that the points $\boldsymbol{\alpha} \in \{0,\pi\}^\beta$ are critical points of the function $\lambda_n(\boldsymbol{\alpha})$: they are the fixed points of the symmetry transformation $\boldsymbol{\alpha} \mapsto -\boldsymbol{\alpha} \pmod{2\pi}$. Henceforth, we will refer to these points as *symmetry points*.

Theorem 2.3 states that the nodal surplus of the eigenfunction at a symmetry point is equal to the Morse index of $\lambda_n(\boldsymbol{\alpha})$ at this point. We now infer from Theorem 3.1 that *none* of the symmetry points are extrema of the eigenvalues $\lambda_n(\boldsymbol{\alpha})$ (with the exception of the eigenvalue $\lambda_1(0,\ldots,0)$, which is always a minimum). Since the $\lambda_n(\boldsymbol{\alpha})$ are continuous functions on the compact torus $(-\pi,\pi]^\beta$, the extrema must be achieved somewhere else.

B. A condition for an internal critical point

Searching for the "missing" extremal points of the functions $\lambda_n(\boldsymbol{\alpha})$, we need to look in the bulk of the fundamental domain of the $\boldsymbol{\alpha}$-space. Critical (extremal) points that are not one of the previously identified symmetry points will be called *internal critical (extremal) points*. A common (and mistaken) assumption is that there are no internal extremal points; it was pointed out in Ref. 31 that such points may occur and explicit examples were constructed in Refs. 31 and 21. Moreover, in the case of mandarin graphs, their occurrence is simply unavoidable; the extrema must be achieved somewhere.

Our search for extremal points is aided by proving a necessary condition that simple internal critical points must obey.

Theorem 3.3. *Let Γ be a graph with first Betti number equal to β and denote by $\boldsymbol{\alpha} \in (-\pi,\pi]^\beta$ the total fluxes through some choice of cycles of the graph that form a basis of its fundamental group. If the eigenvalue $\lambda_n(\boldsymbol{\alpha})$ has an internal critical point $\boldsymbol{\alpha}^*$ (i.e., $\boldsymbol{\alpha}^* \notin \{0,\pi\}^\beta$) and $\lambda_n(\boldsymbol{\alpha}^*)$ is simple, then the eigenfunction corresponding to $\lambda_n(\boldsymbol{\alpha}^*)$ is equal to zero at some vertex of the graph.*

C. The missing extrema are found at touching bands

The necessary condition given in Theorem 3.3 allows us to show that an internal critical point of a mandarin graph must be degenerate. Calling the graph of the function $\lambda_n(\boldsymbol{\alpha})$ a band, we get the following.

Theorem 3.4. *For a generic mandarin graph, all extrema of $\lambda_n(\boldsymbol{\alpha})$, apart from the minimum of $\lambda_1(\boldsymbol{\alpha})$, are achieved at points where two bands touch.*

Figure 2 illustrates the result of the theorem: each pair of consecutive bands touches at two symmetrically located points.

It is well-known that the magnetic spectrum of a graph as a function of the fluxes coincides, by Floquet–Bloch reduction, with the dispersion relation of the Abelian cover of the graph. Here, the phases $\boldsymbol{\alpha}$ take the meaning of the quasi-momenta of the Bloch functions. For a 3-mandarin graph, there are two α-parameters, and a degeneracy in two parameters is typically a conical point (Ref. 1, Appendix 10). The maximal Abelian cover of a 3-mandarin is a honeycomb-like graph, where only the parallel edges are required to have equal length (see Figure 1). The above chain of results shows that typically there are conical ("Dirac") points in the dispersion relation of such a graph between each pair of adjacent bands.

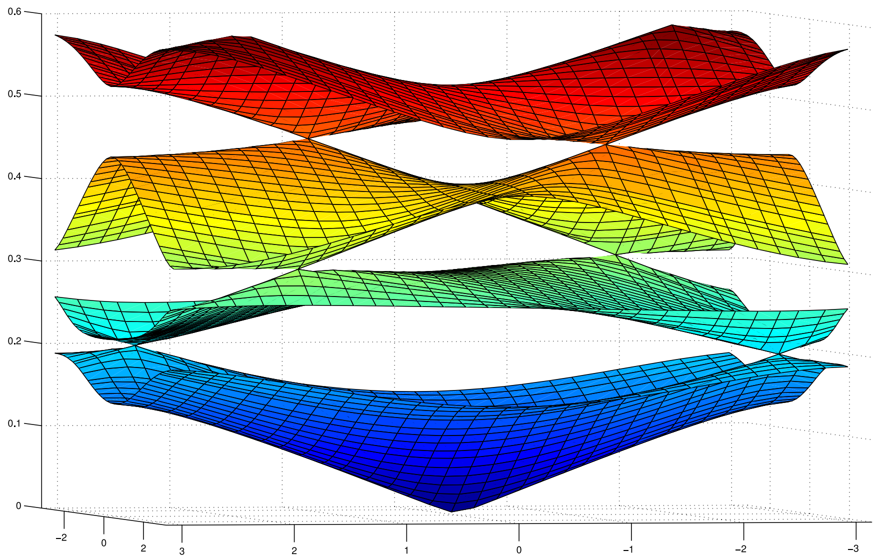

FIG. 2. First four bands of a 3-mandarin graph, as functions of $\beta = 2$ magnetic fluxes. The vertical axis is $k = \sqrt{\lambda}$; in this scale, the bands have comparable sizes.[3] This choice of scale also explains the conical point at the bottom of the lowest band (in contrast, $\lambda_1(\boldsymbol{\alpha})$ is differentiable at $\mathbf{0}$).

IV. INTERLACING AND NODAL COUNT FOR MANDARIN GRAPHS

A. Eigenvalue interlacing

We begin working towards the proof of Theorem 3.1 by establishing some eigenvalue interlacing results, which are heavily based on the inequalities of Ref. 11 (Section 3.1). The following lemma was proved as part of lemma 4.3 of Ref. 5.

Lemma 4.1. Let Γ be a compact connected graph and let $\Lambda = \lambda_n(\Gamma)$ be a simple eigenvalue of Γ with the corresponding eigenfunction f. Let Γ_c be a graph which is the union of $k+1$ connected components such that the following are true:

(1) Γ can be obtained from Γ_c by k operations of gluing a pair of vertices together and adding the parameters χ of their δ-type conditions.
(2) The function f restricted to any of the components of Γ_c is an eigenfunction of that component.

Then,

$$\lambda_{n-1}(\Gamma_c) < \Lambda < \lambda_{n+k+1}(\Gamma_c), \tag{4.1}$$

$$\lambda_n(\Gamma_c) = \lambda_{n+1}(\Gamma_c) = \cdots = \lambda_{n+k}(\Gamma_c) = \Lambda. \tag{4.2}$$

The next lemma we formulate in somewhat greater generality than that which will be necessary in subsequent derivations.

Lemma 4.2. Let Γ be a graph with a Neumann vertex v of degree d whose removal separates the graph into d disjoint subgraphs. We denote its edge set by E_v. Let $r \le d$ be a non-negative integer. For a subset E_D of E_v, with $|E_D| = r$, define Γ_{E_D} to be the modification of the graph Γ obtained by imposing the Dirichlet condition at v for edges from E_D and leaving the edges from $E_v \setminus E_D$ connected at v with the Neumann condition (see Figure 3 for an example). Then,

$$\lambda_{n-1}(\Gamma) \le \min_{|E_D|=r} \lambda_n(\Gamma_{E_D}) \le \lambda_n(\Gamma) \le \max_{|E_D|=r} \lambda_n(\Gamma_{E_D}) \le \lambda_{n+1}(\Gamma). \tag{4.3}$$

Proof. Without loss of generality, we will assume that the eigenvalue $\lambda_n(\Gamma)$ is simple. Indeed, one can resolve multiplicity by an arbitrarily small perturbation of the edge lengths.[28] Since the

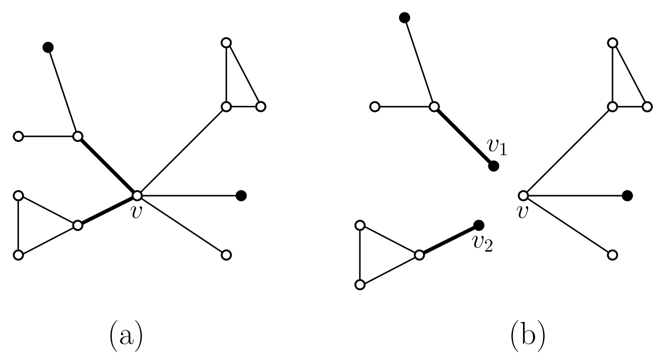

FIG. 3. The original graph Γ, (a), and the resulting graph Γ_{E_D}, (b), when the set E_D comprises of the $r = 2$ edges joining v from the left (shown in thicker lines). Vertices with Neumann conditions are shown as empty circles, and Dirichlet conditions are indicated by filled circles.

nth eigenvalue is a continuous function of the lengths (Ref. 11, Theorem 3.1.11), if the (non-strict) inequality is true for simple eigenvalues, it remains true when passing to the limit of zero perturbation.

The outside equalities: Start from the graph Γ and disconnect any r edges keeping them joined together with the Neumann condition and denoting the resulting graph by Γ'. From Ref. 11 (Theorem 3.1.11), we get

$$\lambda_{n-1}(\Gamma) \le \lambda_n(\Gamma') \le \lambda_{n+1}(\Gamma') \le \lambda_{n+1}(\Gamma).$$

Now, changing the vertex condition from Neumann to Dirichlet disconnects the r edges and results in $\lambda_n(\Gamma') \le \lambda_n\left(\Gamma_{E_D}\right) \le \lambda_{n+1}(\Gamma')$ (Ref. 11, Theorem 3.1.8).

The lower bound for the maximum: We describe the choice of E_D that will fulfill the inequality. We start with the nth eigenfunction f of Γ (normalizing so that $f(v) > 0$). We now choose the r edges e with the largest values of $f_e'(v)$ to be in E_D and get

$$\sum_{e\in E\setminus E_D} f_e'(v) \le 0.$$

Consider f on the graph Γ'_{E_D} obtained by disconnecting the edges from the set E_D at the vertex v. We supply Γ'_{E_D} with conditions that ensure that f is an eigenfunction. Namely, the function f satisfies the δ-type condition at the vertex v with some coefficient $\chi_v \le 0$. At the new vertices v_1, v_2, etc. (see Figure 3), some δ-type conditions are also satisfied. The sum of the parameters of those δ-type conditions together with χ_v is zero. From Lemma 4.1, we have

$$\lambda_n(\Gamma'_{E_D}) = \lambda_n(\Gamma).$$

Now, we modify the conditions of Γ'_{E_D}, increasing χ_v to zero and the δ-type parameters at the new vertices of degree one to ∞ (Dirichlet condition), obtaining the graph Γ_{E_D}. All these operations increase the eigenvalues (Ref. 11, Theorem 3.1.8); in particular,

$$\lambda_n(\Gamma_{E_D}) \ge \lambda_n(\Gamma'_{E_D}) = \lambda_n(\Gamma).$$

The upper bound for the minimum: In this case, we choose the r edges e with the smallest values of $f_e'(v)$ to be in E_D and get

$$\sum_{e\in E\setminus E_D} f_e'(v) \ge 0,$$

and, therefore, $\chi_v \ge 0$. From Lemma 4.1, we have

$$\lambda_{n+r}(\Gamma'_{E_D}) = \lambda_n(\Gamma).$$

Now, we *decrease* χ_v to 0, resulting in

$$\lambda_{n+r}(\Gamma''_{E_D}) \le \lambda_{n+r}(\Gamma'_{E_D}),$$

and then increase the parameters of the new vertices of degree one to ∞, obtaining

$$\lambda_n(\Gamma_{E_D}) \le \lambda_{n+r}(\Gamma''_{E_D}).$$

The desired result is an obvious chaining of the obtained inequalities. □

Remark 4.3. The condition in Lemma 4.2 that removing a vertex of degree d separates the graph into d disjoint subgraphs is necessary for the lower bound in (4.3). This is used in the proof above when applying Lemma 4.1, and indeed there exist examples where the bound does not hold when the condition is not satisfied.

Remark 4.4. In the case of a graph which is "spherically symmetric" around vertex v (i.e., the d disjoint subgraphs obtained by removing the vertex v are identical), we immediately get

$$\lambda_n(\Gamma_{E_D}) = \lambda_n(\Gamma),$$

for all n and E_D. A special case of this is proved and used in a recent work of Demirel-Frank.[19]

Lemma 4.5. Let Γ_{DN} be a tree graph with zero potential, Dirichlet conditions at t of its leaves, and Neumann conditions at all of its other leaves and at all of its internal vertices. Let Γ_{ND} be the same graph with Dirichlet conditions changed to Neumann and vice versa at all leaves. If $k + t - 1 > 0$, then

$$\lambda_k(\Gamma_{DN}) \le \lambda_{k+t-1}(\Gamma_{ND}). \tag{4.4}$$

Remark 4.6. Naively applying the standard interlacing results (see, e.g., Ref. 11 [Theorem 3.1.8]) while changing the condition at each leaf, we would get the weaker result,

$$\lambda_k(\Gamma_{DN}) \le \lambda_{k+t}(\Gamma_{ND}).$$

Remark 4.7. Taking the inequality above with $t = 0$ gives an inequality similar to that known for domains in $\mathbb{R}^d$. In general, if $\Omega \subset \mathbb{R}^d$ is a domain whose Neumann spectrum is discrete, then $\lambda_k^{(N)}(\Omega) \le \lambda_{k-1}^{(D)}(\Omega)$ where the superscript $(N) \setminus (D)$ denotes the Neumann\Dirichlet spectrum.[27,26]

Proof. We start by introducing the spectral counting function,

$$N(\Gamma;\lambda) := |\{n \,|\, \lambda_n(\Gamma) \le \lambda\}|,$$

which we will use to rephrase eigenvalue inequalities. In particular, we have the following equivalence:

$$\lambda_k(\Gamma_1) \le \lambda_{k+s}(\Gamma_2) \text{ for all } k \qquad \Leftrightarrow \qquad N(\Gamma_2;\lambda) \le N(\Gamma_1;\lambda) + s. \tag{4.5}$$

To go from left to right, we observe that if $N(\Gamma_1;\lambda) = n$, then $\lambda < \lambda_{n+1}(\Gamma_1) < \lambda_{n+s+1}(\Gamma_2)$, by definition and left inequality, correspondingly. Applying the definition of N once again, we get $N(\Gamma_2;\lambda) \le n + s$. The left follows from the right by the substitution $\lambda = \lambda_{k+s}(\Gamma_2)$. Using the equivalence above, we write (4.4) as

$$N(\Gamma_{ND};\lambda) \le N(\Gamma_{DN};\lambda) + t - 1, \tag{4.6}$$

which is what we now prove using induction on the number of internal vertices of Γ_{DN}. The starting point is to notice that the lemma holds for intervals (no internal vertices) with either Dirichlet or Neumann conditions at each of their endpoints. Denoting intervals with different types of boundary conditions by I_{DD}, I_{NN}, and $I_{DN} = I_{ND}$, we have

$$\lambda_k(I_{DD}) = \lambda_{k+1}(I_{NN}) = \left(\frac{\pi}{l}k\right)^2,$$

$$\lambda_k(I_{NN}) = \lambda_{k-1}(I_{DD}) = \left(\frac{\pi}{l}(k-1)\right)^2,$$

$$\lambda_k(I_{DN}) = \lambda_k(I_{ND}) = \left(\frac{\pi}{2l}(2k-1)\right)^2,$$

where l is the interval length. Therefore, the lemma holds for an interval, and for such graphs, we even get an equality in (4.4). Assume that the lemma holds for all tree graphs which have no more than M internal vertices. Let Γ_{DN} be a tree graph which satisfies the lemma's conditions and has $M+1$ internal vertices. Let v be an internal vertex of Γ_{DN} with degree d. Note that v has a Neumann condition as it is an internal vertex. We start with $\lambda_k(\Gamma_{DN})$ and apply Lemma 4.2 with $r = d-2$ on the vertex v (choosing E_D which results in the maximal eigenvalue). Denoting the resulting graph by Γ', we have from Lemma 4.2 that

$$\lambda_k(\Gamma_{DN}) \le \lambda_k(\Gamma'), \tag{4.7}$$

or equivalently from (4.5),

$$N(\Gamma'; \lambda) \le N(\Gamma_{DN}; \lambda). \tag{4.8}$$

The resulting graph, Γ', is a union of $d-1$ tree graphs, $\Gamma' = \cup_{i=1}^{d-1}\Gamma_{DN}^{(i)}$. Note that $d-2$ of these graphs have a Dirichlet leaf vertex which originates from v, and therefore these graphs have less internal vertices than Γ_{DN}. In one graph out of the $\Gamma_{DN}^{(i)}$, however, v becomes a Neumann vertex of degree 2 and can be absorbed into the edge. Therefore, this graph also has strictly less internal vertices than Γ_{DN}. Denote by t_i the number of Dirichlet leaves of $\Gamma_{DN}^{(i)}$ and note that

$$\sum_{i=1}^{d-1} t_i = t + d - 2,$$

since we added $d-2$ Dirichlet vertices by splitting the vertex v.

We get by the induction assumption

$$N\left(\Gamma_{ND}^{(i)}; \lambda\right) \le N\left(\Gamma_{DN}^{(i)}; \lambda\right) + t_i - 1, \tag{4.9}$$

where $\Gamma_{ND}^{(i)}$ is the same as $\Gamma_{DN}^{(i)}$, but with Dirichlet and Neumann conditions at all leaves interchanged.

Denoting $\Gamma'' = \cup_{i=1}^{d-1}\Gamma_{ND}^{(i)}$ and using the additivity of the spectral counting function, we get

$$N(\Gamma''; \lambda) = \sum_{i=1}^{d-1} N\left(\Gamma_{ND}^{(i)}; \lambda\right) \le \sum_{i=1}^{d-1}\left(N\left(\Gamma_{DN}^{(i)}; \lambda\right) + t_i - 1\right) = N(\Gamma'; \lambda) + t - 1. \tag{4.10}$$

All that remains is to note that Γ_{ND} is obtained from Γ'' by gluing all vertices which originated from v and are equipped (in Γ'') with Neumann conditions; such gluing increases the eigenvalue (Ref. 11, Theorem 3.1.11), so $\lambda_{k+t-1}(\Gamma'') \le \lambda_{k+t-1}(\Gamma_{ND})$ and therefore,

$$N(\Gamma_{ND}; \lambda) \le N(\Gamma''; \lambda). \tag{4.11}$$

Combining inequalities (4.8), (4.10), (4.11), we get (4.6), which proves the induction step. □

B. Application to nodal count

The interlacing results of Sec. IV A allow one to prove that bi-dendral graphs have anomalous nodal counts: the nodal surplus of a bi-dendral graph with d middle edges is never $\beta = d-1$ or 0 (with the exception of σ_1 which is 0 for all graphs with Neumann conditions). We will prove this fact for a slightly more general setup.

We consider the bi-dendral graph, some of whose middle edges can have an intermediate point v at which anti-Neumann conditions (2.2) are enforced. We can still ask the questions about the number of zeros of the eigenfunction. Note that there is usually a sign change at the above v but *not* a zero. It can also happen that $f|_{e_-}(v) = f|_{e_+}(v) = 0$, but then, on the contrary, f does not change sign at v. The nth *nodal surplus*, as before, is defined as the number of zeros of the nth eigenfunction minus $n-1$.

Placing an anti-Neumann condition at a point on the edge e is unitarily equivalent to placing a magnetic potential that integrates to π on the edge e. In particular, without loss of generality, we can impose each anti-Neumann condition in the middle of the respective edge.

We are now ready to prove Theorem 3.1, which asserts that a generic bi-dendral graph satisfies

$$1 \le \sigma_n \le \beta - 1 = d - 2, \qquad n > 1.$$

Proof of theorem 3.1. Let a be the number of edges on which anti-Neumann conditions are enforced. Since the anti-Neumann conditions are symmetric and can be imposed in the middle of edges (their location along the edge does not affect the eigenvalues nor the nodal count), the graph still has up-down reflection symmetry (see Figure 4, left). Therefore, the spectrum can be decomposed into two halves, even and odd, consisting of eigenvalues whose eigenfunctions are symmetric and those with anti-symmetric eigenfunctions with respect to the reflection.

The symmetric eigenfunctions have Dirichlet conditions at the midpoints of anti-Neumann edges and zero derivative at the midpoints of the rest of the middle edges. There is a one-to-one correspondence between the symmetric eigenfunctions and the eigenfunctions of the upper half of the bi-dendral graph, Γ_{even}, with the corresponding boundary conditions (see Figure 4, right). The antisymmetric eigenfunctions satisfy the opposite conditions and are in correspondence with the eigenfunction of the tree graph Γ_{odd}. Namely, if Γ is a bi-dendral graph, then we have the spectral decomposition $\text{Spec}(\Gamma) = \text{Spec}(\Gamma_{\text{even}}) \cup \text{Spec}(\Gamma_{\text{odd}})$. The resulting pair of trees has opposite vertex conditions on the leaves and therefore fit the description in Lemma 4.5.

Consider the eigenfunction corresponding to $\lambda_k(\Gamma_{\text{even}})$ and assume that this eigenvalue is generic in the spectrum of Γ. As Γ_{even} is a tree graph, this eigenfunction has $k-1$ internal zeros (see Remark 2.4, part 3) and a zeros at the Dirichlet leaves. Its unfolding to the graph Γ therefore has $2(k-1)+a$ zeros. Applying Lemma 4.5 twice for comparison with the graph Γ_{odd} (which has $t = d - a$ Dirichlet leaves), we get

$$\lambda_{k-d+a+1}(\Gamma_{\text{odd}}) < \lambda_k(\Gamma_{\text{even}}) < \lambda_{k+a-1}(\Gamma_{\text{odd}}),$$

the second inequality being valid only when $k + a - 1 > 0$, which is true due to our assumptions ($k > 1$ or $a > 0$). The inequalities above are strict as we assumed $\lambda_k(\Gamma_{\text{even}})$ to be simple when considered as an eigenvalue in the spectrum of Γ. The position of the eigenvalue $\lambda_k(\Gamma_{\text{even}})$ in the spectrum of Γ is equal to the number of eigenvalues of either Γ_{even} or Γ_{odd} that are smaller than or equal to $\lambda_k(\Gamma_{\text{even}})$. From the inequalities above, we deduce that this position is between $2k - d + a + 1$ and $2k - 2 + a$. The nodal surplus is then between

$$2(k-1) + a - (2k - 2 + a - 1) = 1$$

and

$$2(k-1) + a - (2k - d + a + 1 - 1) = d - 2.$$

The calculation for the antisymmetric eigenfunctions is identical modulo the change of a to $d - a$, which has no effect on the final result. □

In the two simplest cases of mandarin graphs (we assume no anti-Neumann conditions), we know all nodal counts exactly.

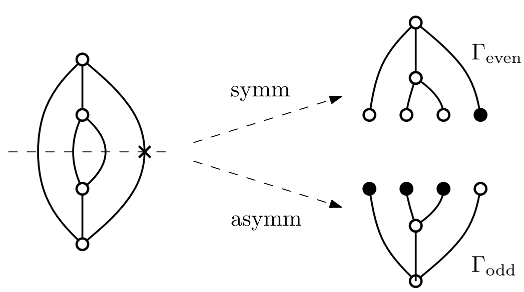

FIG. 4. A bi-dendral graph with an anti-Neumann condition on the fourth middle edge, indicated by a cross. The symmetric eigenfunctions are eigenfunctions of the top tree graph on the right; the antisymmetric ones are the eigenfunctions of the bottom tree graph. Neumann conditions are shown as empty circles and Dirichlet conditions as filled circles.

Corollary 4.8. The nodal surplus count of a mandarin with 3 edges and no magnetic fluxes is $\{0, 1, 1, 1, \ldots\}$. *The nodal surplus count of a mandarin with 4 edges and no magnetic fluxes is* $\{0, 1, 2, 1, 2, 1, \ldots\}$.

Proof. The nodal surplus of the first eigenfunction is always 0 (it does not change sign). The nodal count of 3-mandarin follows immediately from Theorem 3.1 with $d = 3$.

Consider now the 4-mandarin graph. The number of sign changes along *every* edge of the graph must have the same parity: the parity is fully determined by the relative signs of the eigenfunction on the two vertices of the graph. In either cases, the total number of zeros is even. From Theorem 3.1, the (non-trivial) nodal surplus of the 4-mandarin is either 1 or 2, but the even number of zeros forces the alternating pattern. □

V. CRITICAL POINTS OF THE DISPERSION RELATION OF INFINITE QUANTUM GRAPHS

A. Dispersion relation and magnetic Laplacian

Let $\mathbb{G}$ be an infinite $\mathbb{Z}^k$-periodic quantum graph with no magnetic potential. The Schrödinger operator on $\mathbb{G}$ acts as

$$(Hf)(x) = -f''(x) + q(x)f(x), \tag{5.1}$$

where $q(x) \in \mathbb{R}$ is a bounded, periodic, piecewise continuous function that represents electric potential. The conditions on the vertices of $\mathbb{G}$ are assumed to be of δ-type (2.1) and are also periodic.

Choose a fundamental domain $\mathbb{W}$, i.e., a connected subgraph of $\mathbb{G}$ which has one representative of each orbit of $\mathbb{Z}^k$ acting on $\mathbb{G}$ (see Figure 5(a) for an example). We assume that the boundary of $\mathbb{W}$ does not include any vertices of $\mathbb{G}$ (handling the latter would introduce unnecessary notational difficulties).

Denote by $\{s_j\}_{j=1}^k$ some choice of k generators of $\mathbb{Z}^k$ acting on $\mathbb{G}$. We call a pair of vertices, $\left(c_j^+, c_j^-\right)$, belonging to the boundary of $\mathbb{W}$, *quasi-identified* if $s_j\left(c_j^-\right) = c_j^+$ (see Figure 5(b)). We assume that there is only one such pair for each s_j, $j = 1, \ldots, k$. Note that this condition may depend on the choice of the fundamental domain.

Let $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \ldots, \alpha_k)$ and on the graph $\mathbb{W}$ define the operator $H^{\boldsymbol{\alpha}} : \widetilde{H^2}(\mathbb{W}, \mathbb{C}) \to \widetilde{L^2}(\mathbb{W}, \mathbb{C})$, which acts as $-\frac{d^2}{dx^2} + q(x)$ on every edge, along with the conditions

$$\begin{aligned} f(c_j^-) &= e^{i\alpha_j} f(c_j^+), \\ f'(c_j^-) &= -e^{i\alpha_j} f'(c_j^+) \end{aligned} \tag{5.2}$$

at the quasi-identified vertices and the δ-type vertex conditions inherited from the graph $\mathbb{G}$ at all other vertices of $\mathbb{W}$.

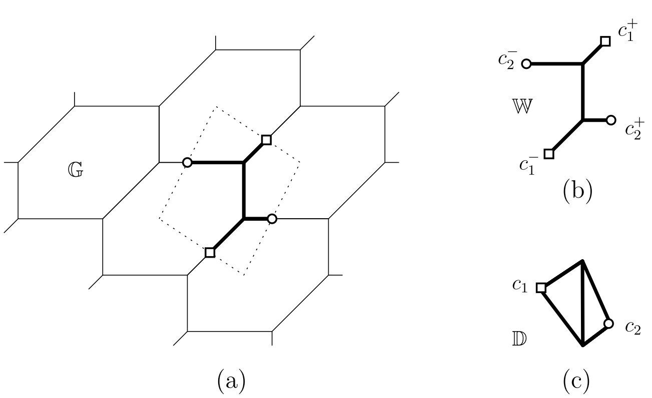

FIG. 5. (a) A $\mathbb{Z}^2$-periodic graph with a chosen fundamental domain; (b) the chosen fundamental domain with quasi-identified vertices marked with the same shape; (c) the graph $\mathbb{D}$ formed by merging the quasi-identified vertices.

By Floquet-Bloch theory (see e.g., Refs. 36 and 11), we know that the spectrum of $\mathbb{G}$ can be found by calculating the eigenvalues of $H^{\boldsymbol{\alpha}}$ and taking the union over all $\boldsymbol{\alpha}$ in the *Brillouin zone*, the torus $(-\pi,\pi]^k$ of all possible values of $\boldsymbol{\alpha}$. In other words,

$$\sigma(H) = \bigcup_{\boldsymbol{\alpha}\in(-\pi,\pi]^k} \sigma(H^{\boldsymbol{\alpha}}).$$

The multi-valued function $\sigma(H^{\boldsymbol{\alpha}})$ is called the *dispersion relation*.

When the operator H is real, as it is in our case, complex conjugation transforms $H^{\boldsymbol{\alpha}}$ into $H^{-\boldsymbol{\alpha}}$, implying that the dispersion relation $\sigma(H^{\boldsymbol{\alpha}})$ is symmetric with respect to the inversion $\boldsymbol{\alpha} \mapsto -\boldsymbol{\alpha}$. The fixed points of this transformation are the vectors $\boldsymbol{\alpha} \in \{0,\pi\}^k$ with all entries equal to either 0 or π. We call these vectors the *symmetry points* of the Brillouin zone. We remark that if $\mathbb{G}$ has additional symmetries, a hierarchy of symmetry points may appear in the Brillouin zone (see Ref. 9 for an example). However, in this work, we reserve the term for the vectors from $\{0,\pi\}^k$ only.

The relation to a magnetic operator on a graph is explicated by the following construction. Beginning with the fundamental domain $\mathbb{W}$, glue the vertices of each quasi-identified pair (c_j^+,c_j^-) to form a new vertex c_j and denote the resulting graph by $\mathbb{D}$ (see Figure 5(c)). When connecting vertices, we do not change the edge lengths. The following easy result can be found, for example, in Ref. 11 (Theorem 2.6.1) or Refs. 34 and 45.

Lemma 5.1. The operator $H^{\boldsymbol{\alpha}}$ is unitarily equivalent to the operator $H^A : \widetilde{H^2}(\mathbb{D},\mathbb{C}) \to \widetilde{L^2}(\mathbb{D},\mathbb{C})$, defined as $-\left(\frac{d}{dx} - iA(x)\right)^2 + q(x)$ on every edge, with the vertex conditions

$$\begin{cases} g(x) \text{ is continuous at } v, \\ \displaystyle\sum_{e\in E_v} \left(\frac{d}{dx_e} - iA(v)\right) g(v) = \chi_v g(v), \qquad \chi_v \in \mathbb{R}, \end{cases}$$

where $A(x)$ is a one-form on $\mathbb{D}$ that satisfies

$$\alpha_j = \int_{c_j^-}^{c_j^+} A(x) \mod 2\pi$$

for any path on $\mathbb{W}$ between c_j^- and c_j^+.

The unitary equivalence is as follows. Choose an arbitrary point, p, on $\mathbb{W}$. If g is an eigenfunction of H^A, then $f := ge^{-i\xi}$ is an eigenfunction of $H^{\boldsymbol{\alpha}}$, where

$$\xi(x) = \int_p^x A(x).$$

Remark 5.2. The magnetic flux α_j is path independent because there is no other magnetic potential on our graph. The integral of $A(x)$ around a cycle in $\mathbb{W}$ (i.e., a cycle that has no magnetic potential) is zero. Since the sign of $A(x)$ (and α_j) depends on direction, the integral around part of a cycle in one direction is equal to the integral around the rest of the cycle traversed in the opposite direction. The same applies to the phase $\xi(x)$.

Lemma 5.1, in particular, shows that the eigenvalues of $H^{\boldsymbol{\alpha}}$ do not depend on the local changes to the choice of the fundamental domain $\mathbb{W}$. Since $|f| = |g|$ and hence $f(x) = 0$ if and only if $g(x) = 0$, we can assume without loss of generality that eigenfunctions are non-zero at c_j, as well as at $c_j^{\pm}$.

Now, we define another operator based on the graph $\mathbb{W}$ by specifying different conditions at the quasi-identified vertices. Let $\boldsymbol{\gamma} = (\gamma_1,\gamma_2,\ldots,\gamma_k)$ and define the operator $H^{\boldsymbol{\gamma}} : \widetilde{H^2}(\mathbb{W},\mathbb{C}) \to \widetilde{L^2}(\mathbb{W},\mathbb{C})$, which acts as $-\frac{d^2}{dx^2} + q(x)$ on every edge, along with the Robin vertex conditions

$$f'(c_j^+) = \gamma_j f(c_j^+),$$
$$f'(c_j^-) = -\gamma_j f(c_j^-)$$

at the quasi-identified vertices and the same conditions as $\mathbb{G}$ at all other vertices. It turns out that extremal points of $\lambda_n(\boldsymbol{\alpha})$ manifest themselves as multiple eigenvalues of $H^{\boldsymbol{\gamma}}$.

Theorem 5.3. *Suppose the infinite periodic quantum graph $\mathbb{G}$ has no magnetic potential and the fundamental domain $\mathbb{W}$ has only one quasi-identified vertex pair in each direction. Let $\lambda_n(\boldsymbol{\alpha})$ have a critical point $\boldsymbol{\alpha}^*$ that is not at a symmetry point of the Brillouin zone (i.e., $\exists j$ such that $\alpha_j^* \neq 0,\pi$), and suppose that the eigenvalue $\lambda_n(\boldsymbol{\alpha}^*)$ is simple with corresponding eigenfunction f.*

Then,

(1) $\gamma_j^* = \frac{f'(c_j^+)}{f(c_j^+)}$ is real for all j,
(2) $\lambda = \lambda_n(\boldsymbol{\alpha}^*)$ is a degenerate eigenvalue of H^{γ^*}, and
(3) if, additionally, $\mathbb{W}$ is a tree, there exists an internal vertex of $\mathbb{W}$, of degree three or higher, such that the eigenfunction f is zero at this vertex.

To prove Theorem 5.3, we first collect some auxiliary useful facts.

B. Critical points of the dispersion relation

Lemma 5.4. If f is an eigenfunction of the operator (5.1), then $\mathrm{Im}(f'(x)\overline{f(x)})$ *is constant on each edge of the graph.*

Proof. We start by calculating the Wronskian of the functions f and $\overline{f}$,

$$\begin{aligned} W(f,\overline{f}) &= f'(x)\overline{f(x)} - f(x)\overline{f'(x)} \\ &= f'(x)\overline{f(x)} - \overline{\overline{f(x)}f'(x)} = 2i\,\mathrm{Im}(f'(x)\overline{f(x)}). \end{aligned}$$

On the other hand, both f and $\overline{f}$ are solutions to the differential equation $-y''(x) + (q(x) - \lambda)y(x) = 0$ on any edge and, by Abel's Theorem, their Wronskian is constant. □

We note that the value of the Wronskian changes from one edge to another. If all vertex conditions are Neumann, the Wronskian defines a flow on the graph. This and other facts about the Wronskian on graphs can be found in Refs. 13 and 48.

In what follows, we will need to differentiate the function $\lambda_n(\boldsymbol{\alpha})$. This is allowed since $\lambda_n(\boldsymbol{\alpha}^*)$ is a simple eigenvalue of $H^{\boldsymbol{\alpha}^*}$, and the function $\lambda_n(\boldsymbol{\alpha})$ is analytic around $\boldsymbol{\alpha} = \boldsymbol{\alpha}^*$[32] (see also Refs. 10 and 11 for a discussion of this fact for quantum graphs).

Lemma 5.5. Suppose that the infinite periodic quantum graph $\mathbb{G}$ satisfies the conditions of Theorem 5.3. If $\boldsymbol{\alpha}^*$ is a critical point of $\lambda_n(\boldsymbol{\alpha})$ and $\lambda_n(\boldsymbol{\alpha}^*)$ is a simple eigenvalue, then the eigenfunction f of $H^{\boldsymbol{\alpha}}$ corresponding to $\lambda_n(\boldsymbol{\alpha}^*)$ satisfies

$$f'(c_j^+)\overline{f(c_j^+)} \in \mathbb{R} \tag{5.3}$$

for all $j = 1,2,\ldots,k$.

Proof. We will show that

$$\frac{\partial\lambda}{\partial\alpha_j} = -2\,\mathrm{Im}\left(f'(c_j^+)\overline{f(c_j^+)}\right), \tag{5.4}$$

which directly implies (5.3) since $\boldsymbol{\alpha}^*$ is a critical point.

By Lemma 5.1, $H^{\boldsymbol{\alpha}}$ and H^A have the same eigenvalues, so

$$\left.\frac{\partial\lambda(\boldsymbol{\alpha})}{\partial\alpha_j}\right|_{\boldsymbol{\alpha}=\boldsymbol{\alpha}^*} = \left.\frac{d}{dt}\lambda(\boldsymbol{\alpha}^* + t\boldsymbol{\delta\alpha}_j)\right|_{t=0} = \left.\frac{d}{dt}\lambda(A^* + tB)\right|_{t=0},$$

where $\boldsymbol{\delta\alpha}_j = (0,\ldots,\delta\alpha_j,\ldots,0)$ and $B(x)$ is any continuous function that satisfies

$$\int_{c_k^-}^{c_k^+} B(x) \mod 2\pi = \begin{cases} \delta\alpha_j & k = j \\ 0 & k \neq j \end{cases}.$$

Denote by e_j the edge of $\mathbb{D}$ which contains c_j. In particular, we choose $\delta\alpha_j = 1$ and a function $B_j(x)$ that is compactly supported on edge e_j near the point c_j and satisfies

$$\int_{c_k^-}^{c_k^+} B_j(x) \mod 2\pi = \delta_{kj}, \tag{5.5}$$

where δ_{kj} is the Kronecker delta function.

Let g_t be an eigenfunction of norm one corresponding to $\lambda(A^* + tB_j)$. We define $g := g_0$ and get from the Hellmann-Feynman Theorem[24] that

$$\frac{d}{dt}\lambda(A^* + tB_j)\bigg|_{t=0} = \left(\frac{d}{dt}H^{A^*+tB_j}\bigg|_{t=0} g, g\right).$$

One can calculate that

$$\begin{aligned}\frac{d}{dt}H^{A^*+tB_j}\bigg|_{t=0} &= -\frac{d}{dt}\left(\frac{d}{dx} - i(A^*(x) + tB_j(x))\right)^2\bigg|_{t=0}\\ &= 2iB_j(x)\frac{d}{dx} + iB_j'(x) + 2A^*(x)B_j(x).\end{aligned}$$

Since $B_j(x)$ is supported on the edge e_j only, we get

$$\begin{aligned}\frac{\partial\lambda(\boldsymbol{\alpha})}{\partial\alpha_j} &= \int_{e_j} iB_j'(x)g(x)\overline{g(x)}\,\mathrm{d}x + \int_{e_j}\left(2iB_j(x)g'(x)\overline{g(x)} + 2A^*(x)B_j(x)|g(x)|^2\right)\,\mathrm{d}x\\ &= \int_{e_j}\left(-iB_j(x)\frac{d}{dx}\left(g(x)\overline{g(x)}\right) + 2iB_j(x)g'(x)\overline{g(x)} + 2A^*(x)B_j(x)|g(x)|^2\right)\,\mathrm{d}x,\end{aligned}$$

using integration by parts (the boundary terms disappear due to the support of $B_j(x)$). Continuing, this gives us

$$\begin{aligned}\frac{\partial\lambda(\boldsymbol{\alpha})}{\partial\alpha_j} &= \int_{e_j} B_j(x)\left[-ig(x)\overline{g'(x)} + A^*(x)g(x)\overline{g(x)} + ig'(x)\overline{g(x)} + A^*(x)g(x)\overline{g(x)}\right]\,\mathrm{d}x\\ &= \int_{e_j} 2B_j(x)\,\mathrm{Im}\left[\left(-g'(x) + iA^*(x)g(x)\right)\overline{g(x)}\right]\,\mathrm{d}x,\end{aligned}$$

where moving from the first line to the second, we use the fact that $A^*(x)$ is real. By Lemma 5.1, we know that since g is an eigenfunction corresponding to $\lambda(A^*)$, $f = ge^{-i\xi}$ is an eigenfunction corresponding to $\lambda(\boldsymbol{\alpha}^*)$, and therefore

$$\mathrm{Im}\left[\left(g'(x) - iA^*(x)g(x)\right)\overline{g(x)}\right] = \mathrm{Im}\left(f'(x)\overline{f(x)}\right).$$

However, by Lemma 5.4, the latter value is a constant on the edge e_j, and using (5.5), we get

$$\frac{\partial\lambda(\boldsymbol{\alpha})}{\partial\alpha_j} = -2\,\mathrm{Im}\left(f'(x)\overline{f(x)}\right)\int_{e_j} B_j(x)\,\mathrm{d}x = -2\,\mathrm{Im}\left(f'(x)\overline{f(x)}\right).$$

□

We are now ready to prove the main theorem of Subsection V A.

Proof of theorem 5.3. Let f be an eigenfunction of $H^{\boldsymbol{\alpha}^*}$ (with $\boldsymbol{\alpha}^*$ not at a symmetry point of the Brillouin zone), and let

$$\gamma_j^* = \frac{f'(c_j^+)}{f(c_j^+)}, \qquad j = 1, \ldots, k.$$

According to Lemma 5.5, all γ_j^*'s are real, and consequently the operator $H^{\boldsymbol{\gamma}^*}$ is self-adjoint and real.

It is easy to see that f is an eigenfunction of $H^{\boldsymbol{\gamma}^*}$. However, f cannot be made real since it satisfies (5.2) and we assumed that there exists j with $\alpha_j^* \neq 0, \pi$. This is not a contradiction only if the real and imaginary parts of f are both eigenfunctions of $H^{\boldsymbol{\gamma}^*}$, in which case λ must be a degenerate eigenvalue of $H^{\boldsymbol{\gamma}^*}$.

Furthermore, if $\mathbb{W}$ is a tree, we can apply (Ref. 11, Corollary 3.1.9), which says that if an eigenvalue of a tree is degenerate, there exists an internal vertex of degree three or higher at which all eigenfunctions from the eigenspace vanish. □

Theorem 3.3 now follows.

Proof of theorem 3.3. Let Γ be a graph with first Betti number equal to β and denote by $\boldsymbol{\alpha} \in (-\pi, \pi]^\beta$ the total fluxes through some choice of cycles of the graph that form a basis of its fundamental group. Therefore, one may cut the graph at β positions to make it a tree graph. The obtained tree graph serves as a fundamental domain $\mathbb{W}$ (with respect to translations) of an infinite $\mathbb{Z}^\beta$-periodic quantum graph, $\mathbb{G}$, as in Theorem 5.3. The statement in Theorem 3.3 now follows from Theorem 5.3(3), realizing that the quasi-momenta of $\mathbb{G}$ are exactly the magnetic fluxes of Γ. □

C. Zeros and touching bands for mandarin graphs

In light of Theorem 5.3, we observe that a special role is played by eigenfunctions that are zero on at least one vertex. We now apply this observation to mandarin graphs.

Proof of theorem 3.4. We will now show that if we have an extremum in the dispersion relation of the mandarin graph, it is due to touching bands.

Assume the contrary: an extremum of $\lambda_n(\boldsymbol{\alpha})$ occurs at $\boldsymbol{\alpha} = \boldsymbol{\alpha}^*$ and $\lambda_n(\boldsymbol{\alpha}^*)$ is simple. The minimum of λ_1 always happens at the point $\boldsymbol{\alpha} = (0, 0, \ldots)$ and we exclude it from further considerations.

First, we argue that the eigenfunction f corresponding to $\lambda_n(\boldsymbol{\alpha}^*)$ must vanish at a vertex of the graph. Indeed, if $\boldsymbol{\alpha}^*$ is not a symmetry point, the claim follows directly from Theorem 3.3. On the other hand, if $\boldsymbol{\alpha}^*$ is a symmetry point and is non-vanishing on the vertices, by combining Theorems 3.1 and 2.3, we conclude that $\boldsymbol{\alpha}^*$ is a saddle point, which contradicts it being an extremum.

Now, without loss of generality, assume that f vanishes on the top vertex of the d-mandarin graph. In addition, f satisfies Neumann conditions there. We can shift the magnetic condition to the top vertex, resulting in

$$f_1(v) = f_2(v) = \cdots = f_d(v) = 0, \tag{5.6}$$

$$e^{i\alpha_1} f_1'(v) + \cdots + e^{i\alpha_{d-1}} f_{d-1}'(v) + f_d'(v) = 0, \tag{5.7}$$

the standard Neumann condition at the bottom vertex, and a non-magnetic operator acting on the edges. Ignoring, for a moment, condition (5.7), we get a standard star graph with d edges and Dirichlet conditions at the boundary vertices. Such a graph, for generic choice of lengths, has eigenfunctions that do not vanish on the central vertex. Hence, we assume that f is not equal to zero at the bottom vertex.

Apply the top-down (vertical) reflection F to the function f (see Figure 4 (left)), followed by complex conjugation. It is immediate to check that the new function, $\overline{Ff}$, satisfies the same eigenvalue problem with $\boldsymbol{\alpha} = \boldsymbol{\alpha}^*$ as the function f. It is, however, a different function: f vanishes on the top vertex and *does not* vanish on the bottom; the function $\overline{Ff}$ does the opposite. We conclude that $\lambda_n(\boldsymbol{\alpha}^*)$ is a multiple eigenvalue. □

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APPENDIX: DISCRETE GRAPHS

In this section, we consider the analogues for discrete graphs of some of the theorems proved above, namely Theorems 3.1, 3.3, and 3.4.

As for the mandarin graphs, one can consider their discrete analogues by placing several intermediate degree-two vertices per edge. However, the anomaly of the nodal count (Theorem 3.1) is only partially exhibited in this case. More specifically, in numerical experiments, we saw that the nodal surplus stays anomalous (i.e., $\sigma_n \neq 0$ and $\sigma_n \neq \beta$) only in the bottom half of the spectrum. Increasing the number of intermediate points per edge, one can approximate any given eigenfunction of the quantum graph, but with a discrete eigenfunction that stays "low" in the spectrum, so these observations do not contradict Theorem 3.1.

We introduce the relevant definitions for discrete graphs in Subsection 1 of the Appendix and discuss the extrema of dispersion relations of infinite periodic discrete graphs in Subsection 2 of the Appendix.

1. Introduction to discrete graphs

Let $\Gamma = (V, E)$ be a simple connected finite graph with vertex set V and edge set E. We define the Schrödinger operator with the potential $q : V \to \mathbb{R}$ by

$$H : \mathbb{C}^{|V|} \to \mathbb{C}^{|V|}, \qquad (Hf)(u) = -\sum_{v\sim u} f(v) + q(u) f(u). \tag{A1}$$

That is, the matrix H is

$$H = Q - C, \tag{A2}$$

where Q is the diagonal matrix of site potentials $q(u)$ and C is the adjacency matrix of the graph. It is perhaps more usual (and physically motivated) to represent the Hamiltonian as $H = Q + L$, where the Laplacian L is given by $L = D - C$ with D being the diagonal matrix of vertex degrees. Since we will not be imposing any restrictions on the potential Q, we absorb the matrix D into Q. The operator H has $|V|$ eigenvalues, which we number in increasing order as before.

The nodal count of a (real) eigenfunction f_n is defined as the number of edges on which the eigenfunction changes sign, i.e.,

$$\phi_n = \left|\{(u,v) \in E \;:\; f_n(u) f_n(v) < 0\}\right|.$$

This count is most relevant for eigenfunctions which do not vanish at vertices. Otherwise, there exists alternative definitions,[14,6] but they are not relevant for the results in this paper.

We define the magnetic Hamiltonian (magnetic Schrödinger operator) on discrete graphs as

$$\left(H^A f\right)(u) = -\sum_{v\sim u} e^{iA_{v,u}} f(v) + q(u) f(u), \tag{A3}$$

with the convention that $A_{v,u} = -A_{u,v}$, which makes H^A self-adjoint. For further details, the reader should consult Refs. 41, 47, 16, and 18.

A sequence of vertices $C = [u_1, u_2, \ldots, u_n]$ is called a *cycle* if each two consecutive vertices, u_j and u_{j+1}, are connected by an edge (u_{n+1} is understood as u_1). The flux through the cycle C is defined as

$$\Phi_C = \left(A_{u_1,u_2} + \cdots + A_{u_{n-1},u_n} + A_{u_n,u_1}\right) \mod 2\pi. \tag{A4}$$

Two operators which have the same flux through every cycle C are unitarily equivalent (by a gauge transformation). Therefore, the effect of the magnetic field on the spectrum is fully determined by β fluxes through a chosen set of basis cycles of the cycle space. We denote them by $\alpha_1,\ldots,\alpha_\beta$ and consider the nth eigenvalue of the graph as a function of $\boldsymbol{\alpha}$.

A result similar to Theorem 2.3 holds for discrete graphs (in fact, discrete graphs were the original context in which the magnetic-nodal connection was established[8,17]). Note that in the discrete version of the theorem, the nodal count should be modified if one considers a symmetric point $\boldsymbol{\alpha}^* \in \{0,\pi\}^\beta$ which differs from zero. The nodal count one should consider in such a case is

$$\phi_n = \left|\{(u,v) \in E \,:\, H_{u,v}(\boldsymbol{\alpha}^*)\, f_n(u) f_n(v) > 0\}\right|,$$

and its surplus, $\phi_n - (n-1)$, equals the Morse index of λ_n at the symmetric point, $\boldsymbol{\alpha}^*$, according to the corresponding theorem.[8,17] Note that this modified nodal count is identical to the one previously defined if $\boldsymbol{\alpha}^* = \mathbf{0}$.

2. Periodic discrete graphs

Let $\mathbb{G}$ be an infinite $\mathbb{Z}^k$-periodic discrete graph such that its Hamiltonian has a $\mathbb{Z}^k$-periodic electric potential, q, and no magnetic potential. We denote by $s_j(v)$ the vertex in $\mathbb{G}$ resulting from shifting the vertex v in the positive jth $\mathbb{Z}^k$-direction. We choose a fundamental domain $\mathbb{W}$ and define two vertices $(v,u) \in \mathbb{W}$ to be the jth *quasi-connected pair* if the vertex $s_j(v)$ is connected to u in $\mathbb{G}$ (see Figure 6). In general, a pair of quasi-connected vertices is not connected in $\mathbb{W}$. We restrict ourselves to graphs $\mathbb{G}$ that have only one quasi-connected pair in each direction, at least for some choice of $\mathbb{W}$.

Let $\boldsymbol{\alpha} = (\alpha_1,\alpha_2,\ldots,\alpha_k)$ and on the fundamental domain $\mathbb{W}$ define the operator $H^{\boldsymbol{\alpha}} = Q - C - M^{\boldsymbol{\alpha}}$, where Q is a diagonal matrix with real entries representing electric potential, C is the connectivity matrix of $\mathbb{W}$, and

$$M^{\boldsymbol{\alpha}}_{(v,u)} = \begin{cases} e^{i\alpha_j} & \text{if } (v,u) \text{ is the } j\text{th quasi-connected pair,} \\ e^{-i\alpha_j} & \text{if } (u,v) \text{ is the } j\text{th quasi-connected pair,} \\ 0 & \text{otherwise.} \end{cases}$$

Similarly, let $\boldsymbol{\gamma} = (\gamma_1,\gamma_2,\ldots,\gamma_k)$ and on $\mathbb{W}$ define the operator $H^{\boldsymbol{\gamma}} = Q - C - M^{\boldsymbol{\gamma}}$ where $M^{\boldsymbol{\gamma}}$ is the diagonal matrix

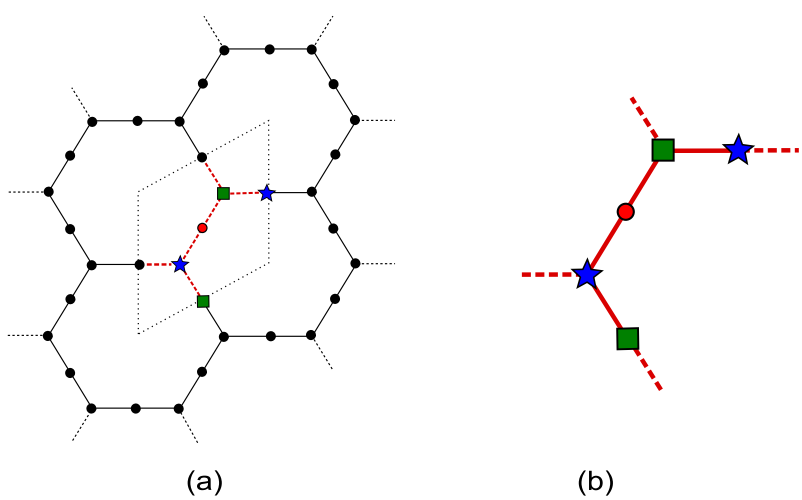

FIG. 6. An infinite $\mathbb{Z}^2$-periodic graph with hexagonal lattice and chosen fundamental domain in box (a); the chosen fundamental domain with quasi-connected vertices marked with the same shape and color (b).

$$M^{\boldsymbol{\gamma}}_{(v,v)} = \begin{cases} \gamma_j & \text{if } (v,u) \text{ is the } j\text{th quasi-connected pair,} \\ \dfrac{1}{\gamma_j} & \text{if } (u,v) \text{ is the } j\text{th quasi-connected pair,} \\ 0 & \text{otherwise.} \end{cases}$$

We are now ready to present the main theorem of this appendix, which is the discrete analogue of Theorem 5.3.

Theorem A.1. *Suppose the infinite periodic discrete graph $\mathbb{G}$ has no magnetic potential and only one quasi-connected vertex pair in each direction, $\lambda_n(\boldsymbol{\alpha})$ has a critical point $\boldsymbol{\alpha}^*$ that is not at a symmetry point of the Brillouin zone (i.e., $\exists j$ such that $\alpha^*_j \neq 0,\pi$), the eigenvalue $\lambda_n(\boldsymbol{\alpha}^*)$ is simple, and the corresponding eigenvector f is non-zero at all quasi-connected vertex pairs. Then,*

(1) $\gamma^*_j = e^{i\alpha^*_j}\frac{f(u)}{f(v)}$ *is real for all j where (v,u) is the jth quasi-connected pair,*
(2) $\lambda = \lambda_n(\boldsymbol{\alpha}^*)$ *is a degenerate eigenvalue of $H^{\boldsymbol{\gamma}^*}$, and*
(3) if, additionally, $\mathbb{W}$ is a tree, there exists an internal vertex of $\mathbb{W}$, of degree three or higher, such that the eigenfunction f is zero at this vertex.

In order to prove Theorem A.1, we establish the following two lemmas.

Lemma A.2. Suppose that the discrete infinite periodic graph $\mathbb{G}$ has no magnetic potential and only one quasi-connected vertex pair in each direction. If $\boldsymbol{\alpha}^*$ is a critical point of $\lambda_n(\boldsymbol{\alpha})$ and $\lambda_n(\boldsymbol{\alpha}^*)$ is a simple eigenvalue, then the eigenvector f corresponding to $\lambda_n(\boldsymbol{\alpha}^*)$ satisfies

$$e^{i\alpha^*_j} f(u)\overline{f(v)} \in \mathbb{R} \qquad \forall j = 1,2,\ldots,k, \tag{A5}$$

where (v,u) is the jth quasi-connected pair.

Proof. Since $\lambda_n(\boldsymbol{\alpha}^*)$ is simple, $\lambda_n(\boldsymbol{\alpha})$ is analytic around the critical point $\boldsymbol{\alpha} = \boldsymbol{\alpha}^*$. Let $f_{\boldsymbol{\alpha}}$ be an eigenvector of norm one corresponding to $\lambda_n(\boldsymbol{\alpha})$. In particular, $f = f_{\boldsymbol{\alpha}^*}$. We have

$$\left(\frac{\partial H^{\boldsymbol{\alpha}}}{\partial \alpha_j}\right)_{(v,u)} = -\left(\frac{\partial M^{\boldsymbol{\alpha}}}{\partial \alpha_j}\right)_{(v,u)} = \begin{cases} -ie^{i\alpha_j} & \text{if } (v,u) \text{ is the } j\text{th quasi-connected pair,} \\ ie^{-i\alpha_j} & \text{if } (u,v) \text{ is the } j\text{th quasi-connected pair,} \\ 0 & \text{otherwise.} \end{cases}$$

Therefore, since $\boldsymbol{\alpha}^*$ is a critical point of $\lambda_n(\boldsymbol{\alpha})$, one can see that

$$\begin{aligned} 0 = \frac{\partial}{\partial \alpha_j}\lambda_n(\boldsymbol{\alpha})\Big|_{\boldsymbol{\alpha}=\boldsymbol{\alpha}^*} = \left(\frac{\partial H^{\boldsymbol{\alpha}^*}}{\partial \alpha_j} f, f\right) &= -ie^{i\alpha^*_j} f(u)\overline{f(v)} + ie^{-i\alpha^*_j} f(v)\overline{f(u)} \\ &= 2\,\mathrm{Im}\left[e^{i\alpha^*_j} f(u)\overline{f(v)}\right], \end{aligned}$$

which completes the proof. □

Lemma A.3. Suppose that $\mathbb{G}$ is a discrete infinite periodic graph and $\boldsymbol{\alpha}^*$ is a critical point of $\lambda_n(\boldsymbol{\alpha})$. If the eigenvector f of $H^{\boldsymbol{\alpha}^*}$ corresponding to $\lambda = \lambda_n(\boldsymbol{\alpha}^*)$ is non-zero at all quasi-connected vertex pairs, then f is also an eigenvector of $H^{\boldsymbol{\gamma}^*}$ corresponding to the same eigenvalue λ where (v,u) is the jth quasi-connected vertex pair and

$$\gamma^*_j = e^{i\alpha^*_j}\frac{f(u)}{f(v)} \in \mathbb{R}.$$

Proof. We will demonstrate that $H^{\boldsymbol{\gamma}^*} f = H^{\boldsymbol{\alpha}^*} f = \lambda f$. Using the definitions of the operators, one can see that this is equivalent to showing

$$H^{\boldsymbol{\gamma}^*} f = (Q-C)f - M^{\boldsymbol{\gamma}^*} f = (Q-C)f - M^{\boldsymbol{\alpha}^*} f = H^{\boldsymbol{\alpha}^*} f = \lambda f,$$

or in other words

$$M^{\boldsymbol{\gamma}^*} f = M^{\boldsymbol{\alpha}^*} f. \tag{A6}$$

Suppose that (v,u) is the jth quasi-connected vertex pair. Then at v, we have

$$(M^{\gamma^*}f)(v) = \gamma_j^* f(v) = e^{i\alpha_j^*}\frac{f(u)}{f(v)}f(v) = e^{i\alpha_j^*}f(u) = (M^{\alpha^*}f)(v).$$

Similarly, at u we have

$$(M^{\gamma^*}f)(u) = \frac{1}{\gamma_j^*}f(u) = e^{-i\alpha_j^*}f(v) = (M^{\alpha^*}f)(u),$$

and at a vertex w which is not in a quasi-connected pair,

$$(M^{\gamma^*}f)(w) = 0 = (M^{\alpha^*}f)(w).$$

□

Proof of theorem A.1. By Lemma A.3, the eigenvector f of H^{α^*} is also an eigenvector of H^{γ^*} (with the same eigenvalue λ). Choose j such that $\alpha_j^* \neq 0,\pi$ (such α_j^* exists by the theorem's conditions). By Lemma A.2,

$$e^{i\alpha_j^*}f(u)\overline{f(v)} \in \mathbb{R}$$

for all j, which means that f has some non-real entries and cannot be made real by scalar multiplication. However, it also means that the operator H^{γ^*} is real and self-adjoint. Therefore, the real and imaginary parts of f must both be linearly independent eigenvectors of H^{γ^*}, which implies that λ is a degenerate eigenvalue of H^{γ^*}.

If $\mathbb{W}$ is a tree, a degenerate eigenvalue can only occur if there exists an internal vertex of degree at least three at which all eigenvectors from the eigenspace vanish.[25] □

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