A LOCAL TEST FOR GLOBAL EXTREMA IN THE DISPERSION RELATION OF A PERIODIC GRAPH

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Abstract. We consider a family of periodic tight-binding models (combinatorial graphs) that have the minimal number of links between copies of the fundamental domain. For this family we establish a local condition of second derivative type under which the critical points of the dispersion relation can be recognized as global maxima or minima. Under the additional assumption of time-reversal symmetry, we show that any local extremum of a dispersion band is in fact its global extremum if the dimension of the periodicity group is three or less, or (in any dimension) if the critical point in question is a symmetry point of the Floquet–Bloch family with respect to complex conjugation. We demonstrate that our results are nearly optimal with a number of examples.

1. Introduction

Wave propagation through periodic media is usually studied using the Floquet–Bloch transform ([AM76, Kuc16]), which reduces a periodic eigenvalue problem over an infinite domain to a parametric family of eigenvalue problems over a compact domain. In the tight-binding approximation often used in physical applications, the wave dynamics is described mathematically in terms of a periodic self-adjoint operator H acting on $\ell^2(\Gamma)$, where Γ is a $\mathbb{Z}^d$-periodic graph (see examples in Figure 1) and d is the dimension of the underlying space. The Floquet–Bloch transform introduces d parameters $\alpha = (\alpha_1, \dots, \alpha_d)$, called *quasimomenta*, which take their values in the torus $\mathbb{T}^d$, called the *Brillouin zone*. The transformed operator $T(\alpha)$ is an $N \times N$ matrix that depends smoothly on α, where N is the number of vertices in a fundamental domain for Γ. The graph of the eigenvalues of $T(\alpha)$, when thought of as a multi-valued function of α, is called the *dispersion relation*. Indexing the eigenvalues in increasing order, we refer to the graph of the the n-th eigenvalue, $\lambda_n(\cdot)$, as the *n-th branch* of the dispersion relation. The range of $\lambda_n(\cdot)$ is called the *n-th spectral band*. The union of the spectral bands is the spectrum of the periodic operator H on $\ell^2(\Gamma)$, the set of wave energies at which the waves can propagate through the medium. The bands edges mark the boundary[1] between propagation and insulation, and are thus of central importance to understanding physical properties of the periodic material. Studying these has applications in condensed matter physics, where periodic tight-binding models of crystalline structure are very common; see [AM76, OPA$^+$19] and references therein.

Naturally, the upper (or lower) edge of the n-th band is the value of the maximum (or minimum) of $\lambda_n(\cdot)$. Since searching for the location of the band edges over the whole torus $\mathbb{T}^d$ can be computationally intensive, the usual approach is to check several points of symmetry and lines between them. However, in dimension greater than one, extrema of the dispersion relation do not have to occur at the symmetry points. This was shown in [HKSW07] using the setting of graphs (both discrete and metric). Figure 2 below shows the example graph

[1] Assuming the bands do not overlap; if the edges for each band are found, this can be easily verified.

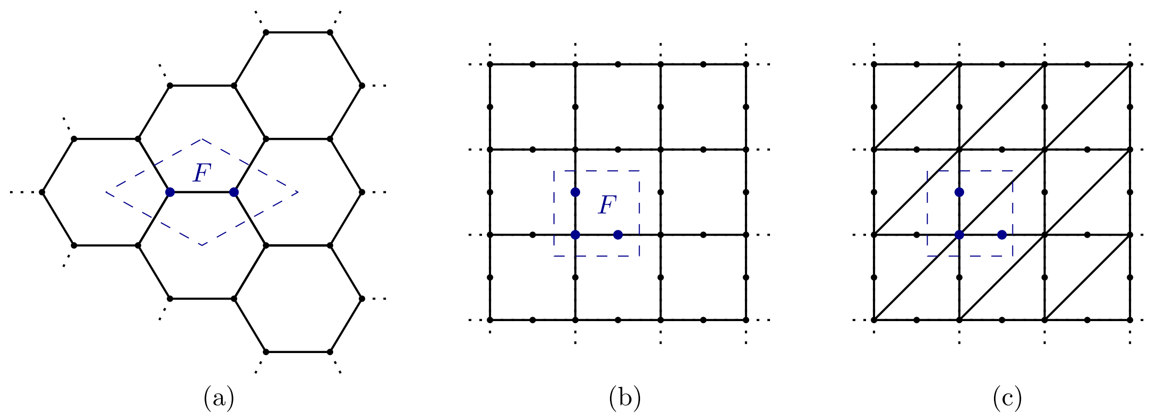

FIGURE 1. The Honeycomb lattice (a) and the Lieb lattice (b) satisfy Definition 1.1, while the augmented Lieb lattice (c) does not. In all figures, the vertices within the dashed line show a possible choice of the fundamental domain F.

found in [HKSW07]. Remarkably, in this work we show that this problem can be overcome on graphs that have "one crossing edge per generator." We now define this concept.

Definition 1.1. Let $\Gamma = (V, \sim)$ be a $\mathbb{Z}^d$-periodic graph (see Definition 2.1), where V denotes the set of vertices and $\sim$ denotes the adjacency relation. Γ is said to have *one crossing edge per generator* if it is connected and there exists a choice of a fundamental domain F such that there are exactly $2d$ adjacent pairs $u \sim v$ with $u \in F$ and $v \in V \setminus F$.

By a fundamental domain F we mean a subset of V containing exactly one representative from each orbit generated by the group action of $\mathbb{Z}^d$. The choice of a fundamental domain is clearly non-unique.

To give some examples, the "one crossing edge per generator" assumption is satisfied by the $\mathbb{Z}^d$ lattice, the graphene lattice shown in Figure 1(a), and the Lieb lattice in Figure 1(b). The graph shown in Figure 1(c) does not satisfy Definition 1.1. For further insight into Definition 1.1 see the discussion around equation (2.1), and see Figure 2 for another example.

In this work we prove that for graphs with one crossing edge per generator, there is a simple local criterion — a variation of the second derivative test — which detects *if a given critical point of* $\lambda_n(\cdot)$ *is a global extremum.* Under additional conditions, this implies that *any local extremum of a band of the dispersion relation is in fact its global extremum.* In a sense, the dispersion relation behaves as if it was a convex function (even though this can never be the case for a continuous function on a torus). As a consequence, even if no local extrema are found among the points of symmetry, it would be enough to run a gradient search-like method.

We now formally state our results. For each $1 \leq n \leq N$, we are interested in the extrema of the continuous function

$$\alpha \mapsto \lambda(\alpha) := \lambda_n\big(T(\alpha)\big).$$

Assuming the eigenvalue is simple[2] at a point α°, $\lambda(\alpha)$ is a real analytic function of α in a neighborhood of α°.

[2]If the eigenvalue is multiple, then two or more bands touch or overlap. This situation is important in applications; there are fast algorithms to find such points [DP09, DPP13, BP20] which lie outside the scope of this work.

The following formulas (see Section 2.2) allow us to look for the critical points of $\lambda(\alpha)$ and to test their *local* character:

$$\nabla\lambda(\alpha^\circ) = B^* f^\circ, \qquad \operatorname{Hess}\lambda(\alpha^\circ) = 2\operatorname{Re} W, \tag{1.1}$$

where

$$W := \Omega - B^*\big(T(\alpha^\circ) - \lambda(\alpha^\circ)\big)^+ B, \tag{1.2}$$

f° is the normalized eigenvector corresponding to the eigenvalue $\lambda(\alpha^\circ)$ of $T(\alpha^\circ)$, B and Ω are correspondingly the $N \times d$ matrix of first derivatives and $d \times d$ matrix of second derivatives of $T(\alpha)$ at $\alpha = \alpha^\circ$ evaluated on f°,

$$B := D\big(T(\alpha) f^\circ\big)\Big|_{\alpha=\alpha^\circ}, \qquad \Omega := \frac{1}{2}\operatorname{Hess}\langle f^\circ, T(\alpha) f^\circ\rangle\Big|_{\alpha=\alpha^\circ}, \tag{1.3}$$

and $\big(T(\alpha^\circ) - \lambda(\alpha^\circ)\big)^+$ denotes the Moore–Penrose pseudoinverse of $T(\alpha^\circ) - \lambda(\alpha^\circ)$.

The textbook second derivative test tells us that a point α° with $B^* f^\circ = 0$ and $\operatorname{Re} W > 0$ is a local minimum. It turns out that a lot more information can be gleaned from the matrix W itself, which may be complex.

Theorem 1.2. *Let Γ be a $\mathbb{Z}^d$-periodic graph with one crossing edge per generator, and let H be a periodic self-adjoint operator acting on $\ell^2(\Gamma)$. Suppose that the n-th branch, $\lambda(\alpha) = \lambda_n\big(T(\alpha)\big)$, of the Floquet–Bloch transformed operator $T(\alpha)$ has a critical point at $\alpha^\circ \in \mathbb{T}^d$. Suppose that $\lambda(\alpha^\circ)$ is a simple eigenvalue of $T(\alpha^\circ)$ and that the corresponding eigenvector f° is non-zero on at least one end of any crossing edge. Let W be the matrix defined in equation* (1.2)*.*

(1) If $W \geq 0$, then $\lambda(\alpha)$ achieves its global minimal value at $\alpha = \alpha^\circ$.
(2) If $W \leq 0$, then $\lambda(\alpha)$ achieves its global maximal value at $\alpha = \alpha^\circ$.

We conjecture that $W \geq 0$ is also a *necessary* condition for the global minimum, and analogously for the global maximum. In Section 5.1.3 we present an example that has a local minimum that is not a global minimum; in this case $\operatorname{Re} W > 0$ while W is sign-indefinite.

We therefore envision the following application of Theorem 1.2: a gradient descent search for a local minimum of $\lambda(\alpha)$ is to be followed by a computation of W according to equation (1.2). If W is non-negative, Theorem 1.2 guarantees that the global minimum is found. If W is sign-indefinite, our conjecture requires the search to continue.

If we additionally assume that the periodic operator H is real symmetric (has "time-reversal symmetry" in physics terminology), the above procedure is simplified substantially. This symmetry of H implies the existence of points $\alpha^* \in \mathbb{T}^d$ such that $\overline{T(\alpha)} = T(\alpha^* - \alpha)$ for all $\alpha \in \mathbb{T}^d$. We denote the set of these points by $\mathcal{C}$ and refer to them informally as "corner points"; for the square parameterization $(-\pi, \pi]^d$ of the Brillouin zone used throughout the paper, we have $\mathcal{C} = \{0, \pi\}^d$.

Theorem 1.3. *Let Γ be a $\mathbb{Z}^d$-periodic graph with one crossing edge per generator, and let H be a periodic real-symmetric operator acting on $\ell^2(\Gamma)$. Suppose that the n-th branch, $\lambda(\alpha) = \lambda_n\big(T(\alpha)\big)$, of the Floquet–Bloch transformed operator $T(\alpha)$ achieves a local extremum at $\alpha^\circ \in \mathbb{T}^d$. Suppose that $\lambda(\alpha^\circ)$ is a simple eigenvalue of $T(\alpha^\circ)$ and that the corresponding eigenvector f° is non-zero on at least one end of any crossing edge. Then, in each of the following circumstances, $\lambda(\alpha^\circ)$ is the global extremal value:*

(1) If $\alpha^\circ \in \mathcal{C}$.
(2) If $d \leq 2$.

(3) If $d = 3$ and the extremum is non-degenerate.

In the setup of Theorem 1.3 the corner points $\mathcal{C}$ are always critical due to the symmetry of the operator. These should be checked first, possibly followed by the general gradient descent search. But in any of the cases specified in the theorem, *the search can stop at the first local minimum found*.

Next, we discuss informally the assumptions of our theorems and the ideas behind the proofs. One crossing edge per generator is a substantial but common assumption: even for $\mathbb{Z}^1$-periodic graphs with real symmetric H, the well-known Hill Theorem is known to fail in the presence of multiple crossing edges, see [EKW10]. In dimension $d = 4$ and higher an internal point may happen to be a local but not a global extremum; see Section 5 for an example. (Since Theorem 1.2 is valid for any d, it follows that the corresponding W is indefinite.)

At the heart of the proof of Theorem 1.2 is a new idea we call the "Lateral Variation Principle."[3] To give a simplified overview,[4] we decompose the operator $T(\alpha)$ as $T(\alpha) = S + R(\alpha)$, where $R(\alpha)$ is a rank-d perturbation and S does not depend on α. It transpires that varying the perturbation $R(\alpha)$ around $\alpha = \alpha^\circ$ yields an eigenvalue function whose Morse index at α° is equal to the spectral shift from S to $T(\alpha)$. Knowing the value of the spectral shift allows us to put a bound on the eigenvalues of $T(\alpha)$, resulting in the estimate

$$\lambda_n\big(T(\alpha^\circ)\big) \leq \lambda_n\big(T(\alpha)\big) \qquad \text{for all } \alpha \in \mathbb{T}^d \tag{1.4}$$

for a local minimum at α°, and the corresponding upper estimate for a local maximum.

The additional assumption of real symmetric H results in $\operatorname{Re} W = W$ if $\alpha^\circ \in \mathcal{C}$. If $\alpha^\circ \notin \mathcal{C}$, then W may be complex. In this case we show that $\det W = 0$; this allows us to estimate the spectrum of W from the spectrum of $\operatorname{Re} W$, but only in low dimensions.

Outline of paper. In Section 2 we present variational formulas for the eigenvalues, and a useful decomposition of the Floquet–Bloch transformed operator. In Section 3 we discuss the relevant spectral/index theory for the lattice models and matrices in question, and provide the proof of Theorem 1.2. In Section 4 we give the proof Theorem 1.3. The main results are demonstrated on some canonical examples on the honeycomb and Lieb lattices in Section 5, where we also provide (counter)-examples showing that when our assumptions are violated the theorems no longer hold. A generalization of the classical Haynsworth formula on the inertia of a Hermitian matrix that is central to our work is given in Appendix A.

Acknowledgements

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[3] In abstract setting of self-adjoint operators this principle is developed in a forthcoming paper [BK19].

[4] This overview corresponds to the proof in Section 3.2 in the simpler case of eigenvector not vanishing anywhere ($P_{\mathrm{Null}(\Omega)} = 0$) while denoting $R(\alpha) = \sum R_j(\alpha_j)$ in equation (3.16). A more precise explanation is given at the beginning of Section 3.2.

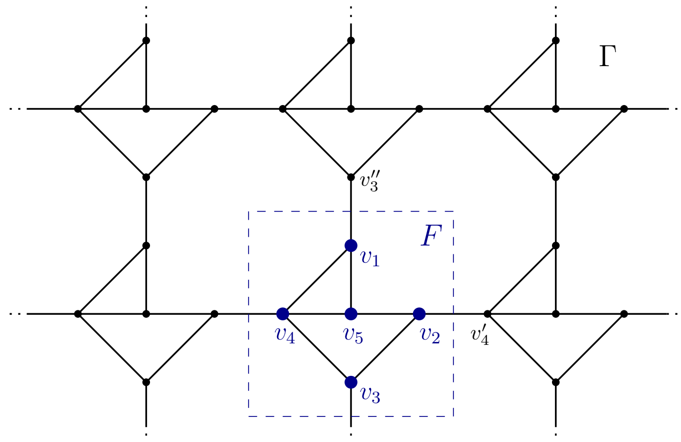

FIGURE 2. An example of a $\mathbb{Z}^2$-periodic graph Γ and its fundamental domain F. If g_1 and g_2 are the horizontal and vertical shifts generating the $\mathbb{Z}^2$ symmetry, then $v_4' = g_1 v_4$ and $v_3'' = g_2 v_3$. The edges with end-vertices (v_2, v_4') and (v_1, v_3'') give rise to the crossing edges, which are (v_2, v_4) and (v_1, v_3).

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2. Basic definitions and local behavior of $\lambda(\alpha)$

In this section we introduce a matrix representation for the Floquet–Bloch transformed operator $T(\alpha)$ (Section 2.1), present a version of the Hellmann–Feyman variational formulas for the n-th eigenvalue branch $\lambda_n\big(T(\alpha)\big)$ (Section 2.2), and give a decomposition formula for $T(\alpha)$ that works under the "one crossing edge per generator" assumption (Section 2.3).

2.1. **Basic definitions.** In this section we introduce a matrix representation for the Floquet–Bloch transformed operator. To do this we first present the notation we shall use for the vertices of the graph and the generators of the group action.

Definition 2.1. A $\mathbb{Z}^d$-*periodic graph* $\Gamma = (V, \sim)$ is a locally finite graph with a faithful cofinite group action by the free abelian group $G = \mathbb{Z}^d$.

In this definition, V is the set of vertices of the graph, and $\sim$ denotes the adjacency relation between vertices. It will be notationally convenient to postulate that $v \sim v$ for any $v \in V$. Each vertex is adjacent to finitely many other vertices ("locally finite"). Any $g \in G$ defines a bijection $v \mapsto gv$ on V which preserves adjacency: $gu \sim gv$ if and only if $u \sim v$ ("action on the graph"). For any $g_1, g_2 \in G$ we have $g_1(g_2 v) = (g_1 g_2)v$ ("group action"). Also, $0 \in G$ is the only element that acts on V as the idenitity ("faithful"). The orbit of v is the subset $\{gv \colon g \in G\} \subset V$ and we assume that there are only finitely many distinct orbits in V ("cofinite").

The "one crossing edge per generator" assumption, introduced in Definition 1.1, is our central assumption on the graph Γ. In addition to the examples of Figure 1, the graph of [HKSW07] in Figure 2 also satisfies the assumption. One can think of such graphs as having been obtained by decorating $\mathbb{Z}^d$ by "pendant" or "spider" decorations [SA00, DKO17]. The terminology "one crossing edge per generator" comes from the following consideration: Under this assumption, there exists a choice of a fundamental domain F such that there are exactly $2d$ adjacent pairs $u \sim v$ with $v \in F$ and $u \in V \setminus F$. In particular, there exists a choice of d generators $\{g_j\}_{j=1}^d$ of G such that

$$u \sim gv, \quad u, v \in F \quad \Longrightarrow \quad g \in \{\mathrm{id}\} \cup \{g_j\} \cup \{g_j^{-1}\}. \tag{2.1}$$

In other words, the fundamental domain is connected only to nearest-neighbors with respect to the generator set.

Definition 2.2. For any generator g_j in $\{g_j\}_{j=1}^d$, there is a unique pair of vertices $u_j, v_j \in F$ such that $u_j \sim g_j v_j$. The pair (u_j, v_j) will be referred to as the *j-th crossing edge.*

We note that while the vertices u_j and v_j may not be adjacent in Γ, they will become adjacent after the Floquet–Bloch transform which we describe next. We also note that u_j and v_j may not be distinct.

Let H be a periodic self-adjoint operator on $\ell^2(\Gamma)$. In the present setting[5]

$$(Hf)_u = \sum_{v \sim u} H_{u,v} f_v, \qquad H_{u,v} \in \mathbb{C}, \qquad H_{v,u} = \overline{H_{u,v}}, \tag{2.2}$$

and

$$H_{gu,gv} = H_{u,v} \quad \text{for any } u, v \in V,\ g \in G. \tag{2.3}$$

We also assume that if u, v are adjacent distinct vertices, then $H_{u,v} \neq 0$.

For a graph with one crossing edge per generator, the transformed operator T is a parameter dependent self-adjoint operator $T(\alpha)\colon \ell^2(F) \to \ell^2(F)$, $\alpha \in \mathbb{T}^d$, acting as

$$(T(\alpha)f)_u = \sum_{\substack{g \in G,\, v \in F \\ gv \sim u}} H_{u,gv} \chi_\alpha(g) f_v, \tag{2.4}$$

where F is a fundamental domain and

$$\chi_\alpha(g) = \begin{cases} 1 & \text{if } g = \mathrm{id}, \\ e^{\pm i\alpha_j} & \text{if } g = g_j^{\pm 1}. \end{cases} \tag{2.5}$$

The function χ_α is the character of a representation of G; we do not need to list its values on the rest of G because of condition (2.1). Continuing to denote by N the number of vertices in a fundamental domain, this means that $T(\alpha)$ may be thought of as an $N \times N$ matrix. For a more general definition of the Floquet–Bloch transform on graphs we refer the reader to [BK13, Chap. 4].

Remark 2.3. It is important to note that we view a periodic graph as a topological object, with an abstract action by an abelian group. In physical applications there is usually a natural geometric embedding of the graph into $\mathbb{R}^d$ and a geometric representation of the periodicity group ("lattice"). The lattice, in turn, determines a particular parameterization of the Brillouin zone $\mathbb{T}^d$ via the "dual lattice." This physical parameterization may differ from the "square lattice" parameterization (2.4)–(2.5) by a linear change in variables α, as illustrated in Figure 3. Our results do not depend on the choice of variables — in particular, the test matrix W can be computed using any parameterization, see Lemma 2.5 below.

[5]Self-adjointness of more general graphs with Hermitian H was studied in [CdVTHT11, Mil11].

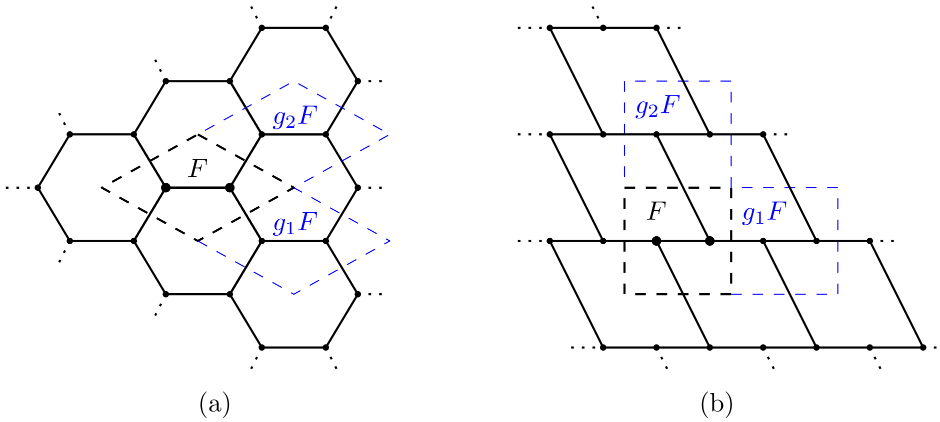


FIGURE 3. (a) “Honeycomb” embedding and (b) “square” embedding of the same graph into $\mathbb{R}^2$. The definition of the Floquet–Bloch transform in the physics literature usually takes the geometry of the embedding into account, but the resulting $T(\alpha)$ would differ only by applying a linear transformation to the variables α (which are then denoted by k).

2.2. **Variational formulas for $\lambda(\alpha)$.** We now recall a multi-dimensional version of the Hellmann–Feyman variational formula that is valid for any family of Hermitian matrices $T(\alpha)$.

Let $T(\alpha)$ be a real analytic family of $N\times N$ Hermitian matrices, parametrized over $\alpha \in \mathbb{T}^d$. Fix a point $\alpha^\circ \in \mathbb{T}^d$ and suppose the n-th eigenvalue $\lambda_n\big(T(\alpha^\circ)\big)$ is simple, with eigenvector f°. For α in a neighborhood of α°, $\lambda_n\big(T(\alpha)\big)$ is simple, and the function $\alpha \mapsto \lambda_n\big(T(\alpha)\big)$ is real analytic; see [Kat76, Section II.6.4]. To streamline notation, we will denote this function by $\lambda(\alpha)$. We are interested in computing the gradient and Hessian of $\lambda(\alpha)$ at $\alpha = \alpha^\circ$.

Let us introduce some notation and conventions. For a scalar function $u(\alpha)$ on $\mathbb{T}^d$, its gradient, ∇u, is a column vector of length d, its differential, Du, is a row vector of length d, and its Hessian, $\operatorname{Hess} u$, is a $d\times d$ symmetric matrix. For vector-valued functions we define D componentwise: if $f\colon \mathbb{T}^d \to \mathbb{R}^N$, then Df is an $N\times d$ matrix-valued function. According to this convention, the matrix B introduced in (1.3) is the $N\times d$ matrix

$$B := D\big(T(\alpha)f^\circ\big)\Big|_{\alpha^\circ} = \begin{bmatrix} \vdots & \vdots & \vdots \\ \frac{\partial}{\partial\alpha_1}(T(\alpha)f^\circ)\Big|_{\alpha^\circ} & \cdots & \frac{\partial}{\partial\alpha_d}(T(\alpha)f^\circ)\Big|_{\alpha^\circ} \\ \vdots & \vdots & \vdots \end{bmatrix}, \tag{2.6}$$

where each $\frac{\partial}{\partial\alpha_j}(T(\alpha)f^\circ)|_{\alpha^\circ}$ is a column vector of size N. We denote by B^* the adjoint of B.

We will regularly use the *Moore–Penrose pseudo-inverse* of a matrix A, denoted A^+. If A is Hermitian, it can be computed as

$$A^+h = \sum_{\lambda_k(A)\neq 0} \frac{1}{\lambda_k(A)}\langle h, f_k\rangle f_k, \tag{2.7}$$

where $\{f_k\}$ is an orthonormal eigenbasis of A with corresponding eigenvalues $\{\lambda_k\}$. With these terms defined, we are thus prepared to state a multi-parameter version of the well known Hellmann–Feynman eigenvalue variational formulas.

Theorem 2.4. *Let $T(\alpha)$ be an analytic family of $N \times N$ Hermitian matrices, parametrized over $\alpha \in \mathbb{T}^d$. Let $\lambda(\alpha^\circ)$ be a simple eigenvalue of $T(\alpha^\circ)$, and let f° be the corresponding eigenvector. For B and W defined in* (1.3) *and* (1.2) *respectively, we have*

$$\nabla\lambda(\alpha^\circ) = D\left\langle f^\circ, T(\alpha) f^\circ\right\rangle\Big|_{\alpha=\alpha^\circ} = B^* f^\circ, \tag{2.8}$$

and

$$\operatorname{Hess}\lambda(\alpha^\circ) = 2\operatorname{Re} W. \tag{2.9}$$

Proof. For fixed $\eta \in \mathbb{R}^d$ define $\hat\lambda(s) = \lambda(\alpha^\circ + s\eta)$, so that

$$\frac{d\hat\lambda}{ds}(0) = \left\langle \nabla\lambda(\alpha^\circ), \eta\right\rangle.$$

On the other hand, the one-dimensional Hellmann–Feynman formula (see [Kat76, Remark II.2.2 (p. 81)]) says

$$\frac{d\hat\lambda}{ds}(0) = \left\langle f^\circ, T^{(1)} f^\circ\right\rangle,$$

where

$$T^{(1)} f^\circ = \frac{d}{ds} T(\alpha^\circ + s\eta) f^\circ\Big|_{s=0} = B\eta.$$

It follows that $\langle \nabla\lambda(\alpha^\circ), \eta\rangle = \langle B^* f^\circ, \eta\rangle$ for all η, which proves (2.8).

Computing similarly for the second derivative, again using [Kat76, Remark II.2.2], we find that

$$\langle \eta, [\operatorname{Hess}\lambda(\alpha^\circ)]\eta\rangle = 2\left[\left\langle f^\circ, T^{(2)} f^\circ\right\rangle - \left\langle T^{(1)} f^\circ, \big(T(\alpha^\circ) - \lambda(\alpha^\circ)\big)^+ T^{(1)} f^\circ\right\rangle\right],$$

where

$$\left\langle f^\circ, T^{(2)} f^\circ\right\rangle = \frac{1}{2}\frac{d^2}{ds^2}\left\langle f^\circ, T(\alpha^\circ + s\eta) f^\circ\right\rangle\Big|_{s=0} = \langle \eta, \Omega\eta\rangle.$$

Substituting $T^{(1)} f^\circ = B\eta$, it follows that

$$\langle \eta, [\operatorname{Hess}\lambda(\alpha^\circ)]\eta\rangle = 2\left\langle \eta, \left(\Omega - B^*\big(T(\alpha^\circ) - \lambda(\alpha^\circ)\big)^+ B\right)\eta\right\rangle = 2\langle \eta, W\eta\rangle$$

for all $\eta \in \mathbb{R}^d$, and hence the symmetric parts of the matrices $\operatorname{Hess}\lambda(\alpha^\circ)$ and $2W$ coincide:

$$\operatorname{Hess}\lambda(\alpha^\circ) + \operatorname{Hess}\lambda(\alpha^\circ)^T = 2(W + W^T).$$

Since the Hessian is real and symmetric, and W is Hermitian, this simplifies to $\operatorname{Hess}\lambda(\alpha^\circ) = W + \overline{W} = 2\operatorname{Re} W$, as claimed. $\square$

We conclude this section by verifying the claim in Remark 2.3 that the sign of W used in Theorem 1.2 can be computed using any parameterization of the torus.

Lemma 2.5. *Let $\phi\colon \mathbb{T}^d \to \mathbb{T}^d$ be a diffeomorphism, and define $\widetilde{T}(k) = T\big(\phi(k)\big)$. Let $\alpha = \alpha^\circ$ be a critical point of a simple eigenvalue $\lambda_n\big(T(\alpha)\big)$. For the matrix W computed from $T(\alpha)$ at α° according to* (1.3)–(1.2), *and $\widetilde{W}$ similarly computed from $\widetilde{T}(k)$ at $k^\circ := \phi^{-1}(\alpha^\circ)$, we have*

$$\widetilde{W} = J^T W J, \tag{2.10}$$

where J is the real invertible Jacobian matrix $J = D\phi(k)\big|_{k=k^\circ}$.

Proof. Applying the chain rule to the definition of $\widetilde{B}$, we get

$$\widetilde{B} := D\left(\widetilde{T}(k)f^\circ\right)\Big|_{k=k^\circ} = D\big(T(\alpha)f^\circ\big)\Big|_{\alpha=\alpha^\circ} D\phi(k)\big|_{k=k^\circ} = BJ.$$

In particular, since α° is a critical point, $\widetilde{B}^* f^\circ = J^T B^* f^\circ = 0$, cf. equation (2.8). Therefore k° is a critical point of the simple eigenvalue $\lambda_n\big(\widetilde{T}(k)\big)$. By a similar calculation, α° is a critical point of the scalar function $\Phi(\alpha) := \langle f^\circ, T(\alpha) f^\circ\rangle$. The Hessian at a critical point transforms under a diffeomorphism as

$$\operatorname{Hess}\Phi(\alpha(k))\big|_{k=k^\circ} = J^T\left(\operatorname{Hess}\Phi(\alpha)\big|_{\alpha=\alpha^\circ}\right)J, \tag{2.11}$$

implying $\widetilde{\Omega} = J^T \Omega J$. Putting it all together implies (2.10). □

We remark that since J is real, (2.10) implies $\operatorname{Re}\widetilde{W} = J^T(\operatorname{Re}W)J$. This could also have been obtained by applying the transformation rule (2.11) to the function $\lambda(\alpha)$, which has Hessian $2\operatorname{Re}W$, according to Theorem 2.4.

2.3. **The decomposition of** $T(\alpha)$**.** Theorem 2.4 is valid for any family $T(\alpha)$ of Hermitian matrices. We now consider the specialized form of the $T(\alpha)$ appearing as the Floquet–Bloch transform of a graph *with one crossing edge per generator*. For a graph satisfying Definition 1.1, there exists a choice of fundamental domain and periodicity generators such that the Floquet–Bloch transformed operator $T(\alpha)$ is given by equation (2.4) and the Brillouin zone $\mathbb{T}^d$ is parameterized by $\alpha \in (-\pi, \pi]^d$. Other physically relevant parameterizations of $T(\alpha)$ may be obtained by a change of variables α; by Lemma 2.5, it is enough to establish our theorems for a single parameterization.

The operator $T(\alpha)$ defined by (2.4) can be decomposed as

$$T(\alpha) = T_0 + \sum_{j=1}^{d} T_j(\alpha_j), \tag{2.12}$$

where T_0 is a constant Hermitian matrix, and each T_j has at most two nonzero entries. More precisely, if $\{g_j\}_{j=1}^d$ are the generators for G, (u_j, v_j) is the j-th crossing edge (see Definition 2.2) and

$$h_j := H_{u_j, g_j v_j},$$

then

$$T_j(\alpha_j) = h_j e^{i\alpha_j}\mathbf{E}_{u_j,v_j} + \overline{h_j} e^{-i\alpha_j}\mathbf{E}_{v_j,u_j}, \tag{2.13}$$

where $\mathbf{E}_{u,v}$ denotes the $N \times N$ matrix with 1 in the u-v entry and all other entries equal to 0. If $u_j \neq v_j$, then $T_j(\alpha_j)$ will have two nonzero entries, appearing in a 2×2 submatrix of the form

$$\begin{bmatrix} 0 & h_j e^{i\alpha_j} \\ \overline{h_j} e^{-i\alpha_j} & 0 \end{bmatrix}.$$

If $u_j = v_j$, then $T_j(\alpha_j)$ has a single nonzero entry, namely $2\operatorname{Re}\left(h_j e^{i\alpha_j}\right)$, on the diagonal.

We now give explicit formulas for B, Ω, and their combinations that will be useful later.

Lemma 2.6. *Let $T(\alpha)$ be as in* (2.12)*. Then for $j = 1, \ldots, d$, the matrix B defined in* (2.6) *has j-th column*

$$\operatorname{col}_j(B) = i\left(h_j e^{i\alpha_j^\circ} f^\circ_{v_j}\mathbf{e}_{u_j} - \overline{h_j} e^{-i\alpha_j^\circ} f^\circ_{u_j}\mathbf{e}_{v_j}\right), \tag{2.14}$$

where $\{\mathbf{e}_u\}_{u=1}^N$ *denotes the standard basis for* $\mathbb{C}^N$*. Consequently,*

$$\frac{\partial \lambda}{\partial \alpha_j}(\alpha^\circ) = -2\,\mathrm{Im}(h_j e^{i\alpha_j^\circ} f_{v_j}^\circ \overline{f_{u_j}^\circ}),$$

and α° *is a critical point of* λ *if and only if*

$$h_j e^{i\alpha_j^\circ} f_{v_j}^\circ \overline{f_{u_j}^\circ} \in \mathbb{R} \tag{2.15}$$

for each $j = 1, \ldots, d$*. In particular, if* $u_j = v_j$ *for some* j*, then* $h_j e^{i\alpha_j^\circ} \in \mathbb{R}$*.*

It was already observed in [BBW15, Lemma A.2] that (2.15) holds at a critical point; we include a proof here for convenience since it follows easily from (2.14).

Proof. Using (2.13) we obtain

$$T_j(\alpha_j) f^\circ = h_j e^{i\alpha_j} f_{v_j}^\circ \mathbf{e}_{u_j} + \overline{h_j} e^{-i\alpha_j} f_{u_j}^\circ \mathbf{e}_{v_j}$$

for each j, and (2.14) follows. Then, from (2.8) and (2.14), we have

$$\frac{\partial \lambda}{\partial \alpha_j}(\alpha^\circ) = \langle \mathrm{col}_j(B), f^\circ \rangle = i\left(h_j e^{i\alpha_j^\circ} f_{v_j}^\circ \overline{f_{u_j}^\circ} - \overline{h_j} e^{-i\alpha_j^\circ} f_{u_j}^\circ \overline{f_{v_j}^\circ} \right) = -2\,\mathrm{Im}(h_j e^{i\alpha_j^\circ} f_{v_j}^\circ \overline{f_{u_j}^\circ}),$$

which completes the proof. ☐

Lemma 2.7. *For* $T(\alpha)$ *as in* (2.12)*, the matrix* Ω *defined in* (1.3) *is diagonal, with*

$$\Omega_{jj} = -\,\mathrm{Re}\left(h_j e^{i\alpha_j^\circ} f_{v_j}^\circ \overline{f_{u_j}^\circ} \right), \tag{2.16}$$

for each $j = 1, \ldots, d$*.*

Proof. As in the proof of Lemma 2.6, we compute

$$\langle T_j(\alpha_j) f^\circ, f^\circ \rangle = h_j e^{i\alpha_j} f_{v_j}^\circ \overline{f_{u_j}^\circ} + \overline{h_j} e^{-i\alpha_j} \overline{f_{v_j}^\circ} f_{u_j}^\circ = 2\,\mathrm{Re}\left(h_j e^{i\alpha_j} f_{v_j}^\circ \overline{f_{u_j}^\circ} \right),$$

and the result follows. ☐

If α° is a critical point, (2.15) and (2.16) together imply that for each $j = 1, \ldots, d$,

$$\Omega_{jj} = -h_j e^{i\alpha_j^\circ} f_{v_j}^\circ \overline{f_{u_j}^\circ} = -\overline{h_j} e^{-i\alpha_j^\circ} \overline{f_{v_j}^\circ} f_{u_j}^\circ. \tag{2.17}$$

In what follows we let J' denote the indices of non-zero diagonal entries of Ω, and let J'' be its complement, namely

$$J' := \{j : f_{u_j}^\circ f_{v_j}^\circ \neq 0\}, \qquad J'' := \{j : f_{u_j}^\circ f_{v_j}^\circ = 0\}. \tag{2.18}$$

Lemma 2.8. *Let* P *be the orthogonal projection onto* $\mathrm{Null}(\Omega)$*. If* α° *is a critical point of* $\lambda(\alpha)$*, then*

$$B\Omega^+ B^* = \sum_{j \in J'} \left(\frac{\Omega_{jj}}{|f_{u_j}^\circ|^2} \mathbf{E}_{u_j,u_j} + h_j e^{i\alpha_j^\circ} \mathbf{E}_{u_j,v_j} + \overline{h_j} e^{-i\alpha_j^\circ} \mathbf{E}_{v_j,u_j} + \frac{\Omega_{jj}}{|f_{v_j}^\circ|^2} \mathbf{E}_{v_j,v_j} \right), \tag{2.19}$$

$$BPB^* = \sum_{j \in J''} |h_j|^2 \left(|f_{v_j}^\circ|^2 \mathbf{E}_{u_j,u_j} + |f_{u_j}^\circ|^2 \mathbf{E}_{v_j,v_j} \right). \tag{2.20}$$

Therefore, $\mathrm{Ran}(BPB^*)$ *is spanned by the vectors*

$$\left\{ \mathbf{e}_{u_j} : f_{u_j}^\circ = 0, f_{v_j}^\circ \neq 0 \right\} \cup \left\{ \mathbf{e}_{v_j} : f_{v_j}^\circ = 0, f_{u_j}^\circ \neq 0 \right\}. \tag{2.21}$$

Remark 2.9. If $u_j = v_j$, the jth summand in (2.19) is identically zero; otherwise it contains a nonzero 2×2 submatrix of the form

$$\begin{bmatrix} \Omega_{jj}|f^\circ_{u_j}|^{-2} & h_j e^{i\alpha^\circ_j} \\ \overline{h_j} e^{-i\alpha^\circ_j} & \Omega_{jj}|f^\circ_{v_j}|^{-2} \end{bmatrix}.$$

The off-diagonal part is precisely the matrix $T_j(\alpha^\circ_j)$ appearing in (2.12); this fact is essential to the proof of Lemma 3.7 below.

Proof. The pseudoinverse Ω^+ is diagonal, with

$$(\Omega^+)_{jj} = \begin{cases} \Omega^{-1}_{jj}, & j \in J', \\ 0, & j \in J''. \end{cases}$$

It follows that

$$B\Omega^+ B^* = \sum_{j\in J'} \Omega^{-1}_{jj} \operatorname{col}_j(B) \operatorname{col}_j(B)^*.$$

Using (2.14) for $\operatorname{col}_j(B)$ and (2.17) for Ω_{jj}, we obtain (2.19).

Similarly, the orthogonal projection P onto $\operatorname{Null}(\Omega)$ is diagonal, with

$$P_{jj} = \begin{cases} 0, & j \in J', \\ 1, & j \in J'', \end{cases}$$

and so

$$BPB^* = \sum_{j\in J''} \operatorname{col}_j(B) \operatorname{col}_j(B)^*.$$

Again, using (2.14) for $\operatorname{col}_j(B)$, (2.20) follows.

Finally, note that the jth summand in (2.20) contains at most one nonzero term, since either $f^\circ_{u_j} = 0$ or $f^\circ_{v_j} = 0$ for each $j \in J''$. In particular, BPB^* is diagonal, and the uth entry is nonzero if and only if either $u = u_j$ for some j such that $f^\circ_{u_j} = 0$ and $f^\circ_{v_j} \neq 0$, or $u = v_j$ for some j with $f^\circ_{v_j} = 0$ and $f^\circ_{u_j} \neq 0$. This establishes (2.21) and completes the proof. □

3. Global properties of $\lambda(\alpha)$: Proof of Theorem 1.2

According to Theorem 2.4, the matrix $\operatorname{Re} W$ (see equation (1.2)) determines if $\lambda(\alpha)$ has a *local* extremum at a given critical point α°. We now turn to establishing Theorem 1.2, which states that the *global* properties of $\lambda(\alpha^\circ)$ are determined by the matrix W itself — without taking its real part. In Section 3.1 we develop some relevant index formulas for W, and in Section 3.2 we use them to prove Theorem 1.2.

3.1. **Index formulas for W.** Let us introduce some notation that will be of use. The inertia of a Hermitian matrix M is defined to be the triple

$$\operatorname{In}(M) := (i_+(M), i_-(M), i_0(M)) =: (i_+, i_-, i_0)_M \tag{3.1}$$

of numbers of positive, negative, and zero eigenvalues of M correspondingly.[6] The second notation will be sometimes used to avoid repetitive specification of the matrix M.

Let $\mathcal{Q}$ be a subspace of the Hilbert space under consideration (which is just $\mathbb{C}^N$ in our case) and let Q denote the orthogonal projection onto $\mathcal{Q}$. For an operator A, we denote by $\big(A\big)_{\mathcal{Q}}$ the operator QAQ^* *considered as an operator on the vector space* $\mathcal{Q}$. We highlight

[6]This particular ordering appears to be traditional in the literature.

that we consider this operator acting on $\mathcal{Q}$ in order to make the dimensions arising in each of our statements below simple to understand.

Lemma 3.1. *Suppose $W = \Omega - B^*A^+B$, where Ω and A are Hermitian matrices of size $d \times d$ and $N \times N$, respectively, and B is an $N \times d$ matrix satisfying*

$$\operatorname{Null}(A) \subset \operatorname{Ran}(B)^\perp = \operatorname{Null}(B^*). \tag{3.2}$$

Let $P = P_{\operatorname{Null}(\Omega)}$ be the orthogonal projection onto $\operatorname{Null}(\Omega)$ and denote $\mathcal{Q} := \operatorname{Null}(BPB^*)$. Define

$$S := \left(A - B\Omega^+ B^*\right)_{\mathcal{Q}},$$

and

$$i_\infty(S) := \operatorname{rk}(BPB^*) = N - \dim(\mathcal{Q}). \tag{3.3}$$

Then,

$$\begin{align} i_-(W) &= i_-(\Omega) + i_-(S) + i_\infty(S) - i_-(A), \tag{3.4}\\ i_0\,(W) &= i_0\,(\Omega) + i_0\,(S) - i_\infty(S) - i_0\,(A), \tag{3.5}\\ i_+(W) &= i_+(\Omega) + i_+(S) + i_\infty(S) - i_+(A) \tag{3.6}\\ &= i_+(\Omega) - i_-(S) - i_0(S) + i_-(A) + i_0(A). \tag{3.7} \end{align}$$

Remark 3.2. If Ω is strictly positive, equation (3.4) simplifies to

$$i_-(W) = i_-(S) - i_-(A).$$

It can be expressed in words as "the Morse index of W is the spectral shift at -0 between S and its positive perturbation $A = S + B\Omega^{-1}B^*$." This idea is further developed in [BK19].

Remark 3.3. The subspace $\mathcal{Q}$ is defined in order to make Ω invertible on $B^*(\mathcal{Q})$. If one considers $A - B\Omega^{-1}B^*$ as a linear relation, then $\mathcal{Q}$ is its regular part and $i_\infty(S)$ is the dimension of its singular part. Informally, $i_\infty(S)$ is the multiplicity of ∞ as an eigenvalue of $A - B\Omega^{-1}B^*$.

Remark 3.4. It follows from the formula for BPB^* given in (2.20) that $i_\infty(S) = \operatorname{rk}(BPB^*)$ is the dimension of the vector space spanned by $\{\operatorname{col}_j(B) : j \in J''\}$; see also (2.21).

Remark 3.5. For $i_+(W)$ we have two forms: equation (3.6) is similar to the previous ones, but equation (3.7) will be directly applicable in our proofs. In addition, the "renormalized" form (3.7) (in the physics sense of cancelling infinities) is the one that retains its meaning if S and A are bounded below but unbounded above, as they would be in generalizing this result to elliptic operators on compact domains.

Proof of Lemma 3.1. The definitions of the matrices W and S are reminiscent of the Schur complement, and so to investigate their indices, it is natural to use the Haynsworth formula [Hay68]. For a Hermitian matrix in block form, $M = \left(\begin{smallmatrix} A & B \\ B^* & C \end{smallmatrix}\right)$ with A *invertible*, the Haynsworth formula states that

$$\operatorname{In}(M) = \operatorname{In}(A) + \operatorname{In}(C - B^*A^{-1}B). \tag{3.8}$$

Several versions of the formula are available for the case when A is no longer invertible (see [Cot74, Mad88]), but the form most suitable for our purposes (equation (3.11) below) we could not find in the literature. For completeness, we provide its proof in Appendix A. Denote by P_A the orthogonal projection onto the nullspace of A and define

$$\mathcal{Q}_A = \operatorname{Null}(B^*P_AB), \qquad i_\infty(M/A) = \operatorname{rk}(B^*P_AB) = \dim(C) - \dim(\mathcal{Q}_A), \tag{3.9}$$

where M/A is the generalized Schur complement of the block A,

$$M/A := C - B^* A^+ B. \tag{3.10}$$

Our generalized Haynsworth formula states that

$$\mathrm{In}(M) = \mathrm{In}(A) + \mathrm{In}_{\mathcal{Q}_A}(M/A) + (i_\infty, i_\infty, -i_\infty)_{M/A}, \tag{3.11}$$

where $\mathrm{In}_{\mathcal{Q}}(X)$ stands for the inertia of X restricted to subspace $\mathcal{Q}$.

The result now follows by a double application of this formula to the block Hermitian matrix

$$M = \begin{pmatrix} A & B \\ B^* & \Omega \end{pmatrix}.$$

Taking the complement with respect to Ω, we find

$$\begin{aligned} \mathrm{In}(M) &= \mathrm{In}(\Omega) + \mathrm{In}_{\mathcal{Q}_\Omega}(M/\Omega) + (i_\infty, i_\infty, -i_\infty)_{M/\Omega} \\ &= \mathrm{In}(\Omega) + \mathrm{In}(S) + (i_\infty, i_\infty, -i_\infty)_S, \end{aligned} \tag{3.12}$$

because $(M/\Omega)_{\mathcal{Q}_\Omega} = S$ and $i_\infty(M/\Omega) = \mathrm{rk}(BP_\Omega B^*) = i_\infty(S)$. On the other hand, taking the complement with respect to A, we find

$$\begin{aligned} \mathrm{In}(M) &= \mathrm{In}(A) + \mathrm{In}_{\mathcal{Q}_A}(M/A) + (i_\infty, i_\infty, -i_\infty)_{M/A} \\ &= \mathrm{In}(A) + \mathrm{In}(W), \end{aligned} \tag{3.13}$$

because (3.2) implies $P_A B = 0$, hence $\mathcal{Q}_A = \mathrm{Null}(B^* P_A B) = \mathbb{C}^d$ and

$$i_\infty(M/A) = \mathrm{rk}(B^* P_A B) = 0.$$

Comparing (3.12) and (3.13), we obtain

$$\mathrm{In}(W) = \mathrm{In}(\Omega) + \mathrm{In}(S) - \mathrm{In}(A) + (i_\infty, i_\infty, -i_\infty)_S,$$

which is precisely (3.4)–(3.6). To obtain (3.7) from (3.6) we use

$$i_\infty(S) = N - \dim(\mathcal{Q}) = \big(i_+(A) + i_-(A) + i_0(A)\big) - \big(i_+(S) + i_-(S) + i_0(S)\big).$$

This completes the proof. ☐

3.2. **Proof of Theorem 1.2.** Letting $\mathcal{Q} = \mathrm{Null}(BP_{\mathrm{Null}(\Omega)}B^*)$ and $A = T(\alpha^\circ) - \lambda(\alpha^\circ)$, we will apply Lemma 3.1 to the matrix

$$S := \big(T(\alpha^\circ) - \lambda(\alpha^\circ) - B\Omega^+ B^*\big)_{\mathcal{Q}}, \tag{3.14}$$

with B and Ω be as in (1.3).

The proof hinges on the fact that we can decompose $\big(T(\alpha)\big)_{\mathcal{Q}} = S + P(\alpha)$, where $P(\alpha)$ is a small-rank perturbation whose signature is determined by Ω. This allows us to bound the spectral shift between S and $T(\alpha)$ in terms of the indices $i_\pm(\Omega)$ and $i_\infty(S)$; we do this in Lemma 3.7. These indices are related to W by Lemma 3.1, and so the hypothesis $W \geq 0$ allows us to put a bound on the eigenvalues of $T(\alpha)$, resulting in the estimate $\lambda_n\big(T(\alpha^\circ)\big) \leq \lambda_n\big(T(\alpha)\big)$ for all $\alpha \in \mathbb{T}^d$.

First, we show that S has the following useful property that will be used here and in the proof of Theorem 1.3.

Lemma 3.6. *If $\lambda(\alpha) = \lambda_n\big(T(\alpha)\big)$ has a critical point at α° and $\lambda(\alpha^\circ)$ is a simple eigenvalue, then* 0 *is an eigenvalue of S as defined in* (3.14).

Proof. Theorem 2.4 implies $B^* f^\circ = 0$, so $f^\circ \in \mathcal{Q}$ and hence

$$Sf^\circ = \big(T(\alpha^\circ) - \lambda(\alpha^\circ)\big) f^\circ = 0.$$

$\square$

Next, we prove a version of the Weyl bracketing inequality for S and $T(\alpha)$.

Lemma 3.7. *Suppose that $\lambda(\alpha) = \lambda_n\big(T(\alpha)\big)$ has a critical point at α° and that $\lambda(\alpha^\circ)$ is a simple eigenvalue. Let f° be the corresponding eigenvector and assume that f° is non-zero on at least one end of any crossing edge (see Definition 2.2). Then, for any $\alpha \in \mathbb{T}^d$ the eigenvalues of $T(\alpha)$ and S, as defined in (3.14), are related by*

$$\lambda_{n-i_-(\Omega)-i_\infty(S)}(S) \le \lambda_n\big(T(\alpha)\big) - \lambda(\alpha^\circ) \le \lambda_{n+i_+(\Omega)}(S). \tag{3.15}$$

Proof. We recall that the crossing edges for the graph are denoted by (u_j, v_j) with $j = 1, \ldots, d$ (see Definition 2.2). Let $J' = \{j : f^\circ_{u_j} f^\circ_{v_j} \neq 0\}$ and consider the matrix

$$S'(\alpha) := T(\alpha) - \lambda(\alpha^\circ) - \sum_{j \in J'} R_j(\alpha_j), \tag{3.16}$$

with

$$R_j(\alpha_j) := \frac{\Omega_{jj}}{|f^\circ_{u_j}|^2}\mathbf{E}_{u_j,u_j} + h_j e^{i\alpha_j}\mathbf{E}_{u_j,v_j} + \overline{h_j} e^{-i\alpha_j}\mathbf{E}_{v_j,u_j} + \frac{\Omega_{jj}}{|f^\circ_{v_j}|^2}\mathbf{E}_{v_j,v_j}. \tag{3.17}$$

We note that at the point $\alpha = \alpha^\circ$ the sum of $R_j(\alpha_j^\circ)$ matches the expression for $B\Omega^+B^*$ obtained in Lemma 2.8. If $u_j \neq v_j$, the matrix $R_j(\alpha_j)$ has four nonzero entries, appearing in a 2×2 submatrix of the form

$$\begin{bmatrix} \Omega_{jj}|f^\circ_{u_j}|^{-2} & h_j e^{i\alpha_j} \\ \overline{h_j} e^{-i\alpha_j} & \Omega_{jj}|f^\circ_{v_j}|^{-2} \end{bmatrix}. \tag{3.18}$$

If $u_j = v_j$, then $R_j(\alpha_j)$ has a single nonzero entry,

$$2\,\mathrm{Re}\left(h_j e^{i\alpha_j} - h_j e^{i\alpha_j^\circ}\right), \tag{3.19}$$

appearing on the diagonal.

The matrices $R_j(\alpha_j)$ have several crucial properties. First, they are the minimal rank perturbations that remove from $S'(\alpha)$ any dependence on the α_j with $j \in J'$. Second, once restricted to $\mathcal{Q} = \mathrm{Null}(BP_{\mathrm{Null}(\Omega)}B^*)$, the dependence on the remaining α_j is eliminated and $S'(\alpha)$ turns into S defined in (3.14). More precisely, we will now show that

$$S = \big(S'(\alpha)\big)_{\mathcal{Q}}. \tag{3.20}$$

From (2.13), (2.19) and (3.17) we obtain

$$\begin{aligned}\sum_{j \in J'} R_j(\alpha_j) &= \sum_{j \in J'} \big[T_j(\alpha_j) - T_j(\alpha_j^\circ)\big] + B\Omega^+B^* \\ &= T(\alpha) - T(\alpha^\circ) - \sum_{j \notin J'} \big[T_j(\alpha_j) - T_j(\alpha_j^\circ)\big] + B\Omega^+B^*,\end{aligned}$$

and so

$$S'(\alpha) = T(\alpha^\circ) - \lambda(\alpha^\circ) - B\Omega^+B^* + \sum_{j \in J''} \big[T_j(\alpha_j) - T_j(\alpha_j^\circ)\big], \tag{3.21}$$

where $J'' = \{j : f^\circ_{u_j} f^\circ_{v_j} = 0\}$. Each of the summands $T_j(\alpha_j) - T_j(\alpha_j^\circ)$ is a linear combination of the basis matrices $\mathbf{E}_{u_j,v_j}$ and $\mathbf{E}_{v_j,u_j}$. Fix an arbitrary $j \in J''$. Since f° is non-zero on at least one end of any crossing edge, we may assume without loss of generality that $f^\circ_{u_j} = 0$ and $f^\circ_{v_j} \neq 0$. Then from (2.21) we have $\mathbf{e}_{u_j} \in \operatorname{Ran}(BPB^*) = \operatorname{Null}(BPB^*)^\perp = \mathcal{Q}^\perp$, so $Q\mathbf{e}_{u_j} = 0$, where Q is the projection operator onto $\mathcal{Q}$. This implies $Q\mathbf{E}_{u_j,v_j} = 0$ and $\mathbf{E}_{v_j,u_j}Q^* = 0$ and therefore

$$Q\mathbf{E}_{u_j,v_j}Q^* = Q\mathbf{E}_{v_j,u_j}Q^* = 0.$$

It follows that all the summands in (3.21) with $j \in J''$ vanish when conjugated by the projection matrix Q. This completes the proof of (3.20).

We now relate the eigenvalues of $T(\alpha)$ and $S'(\alpha)$ by computing the signature of the $R_j(\alpha_j)$ perturbations. If $u_j \neq v_j$, it follows from (2.17) that the determinant of the matrix (3.18) vanishes, and so it has rank one, with signature given by the sign of Ω_{jj}.

On the other hand, if $u_j = v_j$, the matrix has at most one non-zero entry. From Lemma 2.6 we have $h_j e^{i\alpha^\circ_j} \in \mathbb{R}$, and so

$$\operatorname{Re}\left(h_j e^{i\alpha_j} - h_j e^{i\alpha_j^\circ}\right) = h_j e^{i\alpha_j^\circ} \operatorname{Re}\left(e^{i(\alpha_j - \alpha_j^\circ)} - 1\right) = h_j e^{i\alpha_j^\circ}[\cos(\alpha_j - \alpha_j^\circ) - 1].$$

Since $\cos(\alpha_j - \alpha_j^\circ) < 1$ for $\alpha_j \neq \alpha_j^\circ$ and $\Omega_{jj} = -h_j e^{i\alpha_j^\circ}|f^\circ_{u_j}|^2$, we conclude that $R_j(\alpha_j)$ has the same sign as Ω_{jj} provided $\alpha_j \neq \alpha_j^\circ$.

Summing over all $j \in J'$, we conclude that $T(\alpha) - \lambda(\alpha^\circ) - S'(\alpha)$ has at most $i_-(\Omega)$ negative and at most $i_+(\Omega)$ positive eigenvalues. It follows from the classical Weyl interlacing inequality that

$$\lambda_{n-i_-(\Omega)}\big(S'(\alpha)\big) \leq \lambda_n\big(T(\alpha)\big) - \lambda(\alpha^\circ) \leq \lambda_{n+i_+(\Omega)}\big(S'(\alpha)\big) \tag{3.22}$$

for all $\alpha \in \mathbb{T}^d$.

Now, applying the Cauchy interlacing inequality (for submatrices or, equivalently, for restriction to a subspace) to $S'(\alpha)$ and $S = \big(S'(\alpha)\big)_{\mathcal{Q}}$, we get

$$\lambda_{m-i_\infty(S)}(S) \leq \lambda_m\big(S'(\alpha)\big) \leq \lambda_m(S)$$

for all $\alpha \in \mathbb{T}^d$. Combining this with (3.22), we obtain the result. □

Remark 3.8. The hypothesis that f° does not vanish identically on any crossing edge, which was used in the proof of (3.20), can be weakened slightly. If $f^\circ_{u_j} = f^\circ_{v_j} = 0$ for some j, the proof would still hold if we can show that $\mathbf{e}_{u_j}$ or $\mathbf{e}_{v_j}$ belong to the range of BPB^*. The latter would hold if there exists another index k with u_k coinciding with either u_j or v_j and with $f^\circ_{v_k} \neq 0$.

We are now ready to prove Theorem 1.2, which for convenience we restate here in an equivalent form.

Theorem 3.9. *Let $T(\alpha)$ be as in (2.12) and W be as defined in (1.2). Suppose $\lambda(\alpha) = \lambda_n\big(T(\alpha)\big)$ has a critical point at α° such that $\lambda(\alpha^\circ)$ is simple and that the corresponding eigenvector f° is non-zero on at least one end of any crossing edge.*

If $i_-(W) = 0$, then

$$\lambda(\alpha^\circ) \leq \lambda(\alpha) \qquad \text{for all } \alpha \in \mathbb{T}^d, \tag{3.23}$$

i.e. $\lambda(\alpha)$ achieves its global minimum at α°.

If $i_+(W) = 0$, then

$$\lambda(\alpha) \leq \lambda(\alpha^\circ) \qquad \text{for all } \alpha \in \mathbb{T}^d. \tag{3.24}$$

i.e. $\lambda(\alpha)$ achieves its global maximum at α°.

Proof. Let

$$A := T(\alpha^\circ) - \lambda(\alpha^\circ).$$

Consider first the case $i_-(W) = 0$. From Lemma 3.1, equation (3.4) we get

$$0 = i_-(\Omega) + i_-(S) + i_\infty(S) - i_-(A),$$

and hence, using $i_-(A) = n - 1$,

$$n - i_-(\Omega) - i_\infty(S) = i_-(S) + 1.$$

By the definition of negative index, $\lambda_{i_-(S)+1}(S)$ is the smallest non-negative eigenvalue of S, which is 0 by Lemma 3.6. Then applying Lemma 3.7, we get

$$0 = \lambda_{i_-(S)+1}(S) = \lambda_{n-i_-(\Omega)-i_\infty(S)}(S) \le \lambda_n\big(T(\alpha)\big) - \lambda(\alpha^\circ),$$

completing the proof of inequality (3.23).

For the other case, $i_+(W) = 0$, we use Lemma 3.2, equation (3.7), together with the observation that

$$i_-(A) + i_0(A) = n,$$

because $\lambda(\alpha^\circ)$ is simple, to obtain

$$n + i_+(\Omega) = i_-(S) + i_0(S).$$

Now observe that $\lambda_{i_-(S)+i_0(S)}(S)$ is the largest non-positive eigenvalues of S, which is 0 by Lemma 3.6. We then use the upper estimate in Lemma 3.7 to obtain

$$\lambda_n\big(T(\alpha)\big) - \lambda(\alpha^\circ) \le \lambda_{n+i_+(\Omega)}(S) = \lambda_{i_-(S)+i_0(S)}(S) = 0,$$

which completes the proof of (3.24). ∎

4. Real symmetric case: Proof of Theorem 1.3

From Theorems 2.4 and 1.2, we have the implications

$$\text{local minimum at } \alpha^\circ \quad \Longrightarrow \quad \operatorname{Re} W \ge 0,$$

and

$$W \ge 0 \quad \Longrightarrow \quad \text{global minimum at } \alpha^\circ,$$

and similarly for maxima. We now restrict our attention to the case of real symmetric H, with the goal of relating the spectrum of W to the spectrum of its real part. At corner points this is always possible, since W ends up being real. At interior points, W may be complex. However, for $d \le 3$ the real part contains enough information to control the spectrum of the full matrix. This is no longer true when $d \ge 4$. These observations are at the heart of Theorem 1.3, whose proof we divide into two parts. Section 4.1 deals with corner points, while Section 4.2 deals with interior ones.

As in the rest of the manuscipt, we fix an arbitrary $1 \le n \le N$ and consider $\lambda_n\big(T(\alpha)\big)$ as a function of α, which we denote by $\lambda(\alpha)$.

4.1. **Corner points: Proof of Theorem 1.3, case (1).** The following lemma, combined with Theorems 1.2 and 2.4, yields the proof of Theorem 1.3(1).

Lemma 4.1. *Assume $T(\alpha)$ is the Floquet–Bloch transform of a real symmetric operator H. Let $\alpha^\circ \in \mathcal{C} = \{0,\pi\}^d$ and assume that $\lambda(\alpha^\circ)$ is simple. Then, α° is a critical point of $\lambda(\alpha)$ and the corresponding W is real, i.e. $W = \operatorname{Re} W$.*

Proof. At a corner point α° each $e^{i\alpha_j^\circ}$ is real. Therefore $T(\alpha^\circ)$ is a real symmetric matrix, so we can assume that the eigenvector f° is real. It then follows from (2.14) that the matrix B is purely imaginary, and hence the vector $B^* f^\circ$ is as well. On the other hand, $B^* f^\circ$ is real as the gradient of a real function (see Theorem 2.4), so we conclude that $B^* f^\circ = 0$ and hence α° is a critical point.

Since Ω is real (as the Hessian of a real function, see (1.3)), $T(\alpha^\circ) - \lambda(\alpha^\circ)$ is real, and B is imaginary, we therefore find that $W = \Omega - B^*\big(T(\alpha^\circ) - \lambda(\alpha^\circ)\big)^+ B$ is real. □

Remark 4.2. The condition of H being real can be relaxed. If the matrix T_0 appearing in the decomposition (2.12) is real, then any complex phase in the coefficient h_j can be absorbed as a shift of the corresponding α_j. Of course, that would shift the location of the "corner points."

The condition of real T_0 may turn out to hold after a "change of gauge" transformation. Combinatorial conditions for the existence of a suitable gauge and a suitable choice of the fundamental domain were investigated in [HS99, KS17, KS18].

Remark 4.3. On lattices whose fundamental domain is a tree, one can also test the local character of the extremum at $\alpha^\circ \in \mathcal{C}$ by counting the sign changes of the corresponding eigenvector. More precisely, assuming f° is the n-th eigenfunction of $T(\alpha^\circ)$ and is non-zero on any v, the Morse index of the critical point $\alpha^\circ \in \mathcal{C}$ was shown in [Ber13, CdV13] (see also [BBW15, Appendix A.1]) to be equal to $\phi_n - (n-1)$, where

$$\phi_n = \#\{(u,v)\colon T_{u,v}(\alpha^\circ) f_u^\circ f_v^\circ > 0\}.$$

4.2. **Interior points: Proof of Theorem 1.3, cases (2) and (3).** Next we deal with the case that $\alpha^\circ \in \mathbb{T}^d$ is not a corner point. In this case W is in general complex, so $\operatorname{Hess} \lambda(\alpha^\circ) = 2 \operatorname{Re} W$ may not contain enough information to determine the indices $i_\pm(W)$. However, it turns out that if $\alpha^\circ \in \mathbb{T}^d$ is not a corner point, then 0 must be an eigenvalue of W. This provides enough information to obtain the desired conclusion in dimensions $d = 2$ and 3, as claimed in cases (2) and (3) of Theorem 1.3.

Theorem 4.4. *Assume $T(\alpha)$ is the Floquet–Bloch transform of a real symmetric operator H and α° is a critical point of $\lambda(\alpha)$, such that $\lambda(\alpha^\circ)$ is simple and the corresponding eigenvector f° is non-zero on at least one end of each crossing edge (see Definition 2.2). Then, $\alpha^\circ \in \mathbb{T}^d \setminus \{0,\pi\}^d$ implies $i_0(W) \geq 1$.*

This theorem shows an intriguing contrast between W and the Hessian of $\lambda(\alpha)$, the latter of which is the real part of W and is conjectured to be generically non-degenerate (see [DKS19] for a thorough investigation of diatomic graphs and [FK18] for a positive result elliptic operators on $\mathbb{R}^2$).

For the proof, we will need the following observation.

Lemma 4.5. *Under the assumptions of Theorem 4.4, the matrix S defined in* (3.14) *has real entries.*

Proof. We recall that the crossing edges for the graph are denoted by (u_j, v_j) with $j = 1, \dots, d$ (see Definition 2.2). We also continue to refer to J' and J'' as defined in (2.18). From the decomposition (2.12) we have

$$T(\alpha^\circ) - \lambda(\alpha^\circ) = T_0 - \lambda(\alpha^\circ) + \sum_{j \in J'} T_j(\alpha_j^\circ) + \sum_{j \in J''} T_j(\alpha_j^\circ),$$

with T_0 and $\lambda(\alpha^\circ)$ real. It was shown in the proof of Lemma 3.7 that the summands with $j \in J''$ vanish when conjugated by the orthogonal projection Q onto $\mathcal{Q} = \mathrm{Null}(BP_{\mathrm{Null}(\Omega)}B^*)$. Hence, it is enough to show that

$$\sum_{j \in J'} T_j(\alpha_j^\circ) - B\Omega^+ B^*$$

is real. Using (2.19), we can write this as a sum of terms of the form

$$\begin{bmatrix} 0 & h_j e^{i\alpha_j^\circ} \\ \overline{h_j} e^{-i\alpha_j^\circ} & 0 \end{bmatrix} - \begin{bmatrix} \Omega_{jj}|f_{u_j}^\circ|^{-2} & h_j e^{i\alpha_j^\circ} \\ \overline{h_j} e^{-i\alpha_j^\circ} & \Omega_{jj}|f_{v_j}^\circ|^{-2} \end{bmatrix} = - \begin{bmatrix} \Omega_{jj}|f_{u_j}^\circ|^{-2} & 0 \\ 0 & \Omega_{jj}|f_{v_j}^\circ|^{-2} \end{bmatrix}$$

which have real entries by Lemma 2.7. □

Proof of Theorem 4.4. We first rewrite equation (3.5) of Lemma 3.2 as a sum of non-negative terms,

$$i_0(W) = (i_0(\Omega) - i_\infty(S)) + (i_0(S) - 1),$$

with S as defined in (3.14) and $i_0(A) = i_0\big(T(\alpha^\circ) - \lambda(\alpha^\circ)\big) = 1$. The first term is non-negative because $i_0(\Omega) = \mathrm{rk}(P) \geq \mathrm{rk}(BPB^*) = i_\infty(S)$, and the second term is non-negative by Lemma 3.6.

First, suppose the real and imaginary parts of f° are linearly independent. From Lemma 3.6 we have $f^\circ \in \mathcal{Q}$. Because S is real, $\mathrm{Re}\, f^\circ$ and $\mathrm{Im}\, f^\circ$ are linearly independent null-vectors of S, so we have $i_0(S) \geq 2$ and hence $i_0(W) \geq 1$. Thus, for the remainder of the proof we can assume that the real and imaginary parts of f° are linearly dependent. Multiplying by a complex phase, this is the same as assuming that f° is real.

Since α° is not a corner point, we can assume, without loss of generality, that $\alpha_1 \notin \{0, \pi\}$. Using (2.15), the criticality of α° implies that $f_{u_1}^\circ f_{v_1}^\circ e^{i\alpha_1^\circ} \in \mathbb{R}$, and therefore $f_{u_1}^\circ f_{v_1}^\circ = 0$. Since f° is non-zero on at least one end of any crossing edge, we may assume that $f_{u_1}^\circ = 0$ and $f_{v_1}^\circ \neq 0$. From (2.14) we see that the first column of B has a single nonzero entry, in the u_1 component.

From the decomposition (2.12) we have $T(\alpha^\circ)_{u_1,v_1} = h_1 e^{i\alpha_1^\circ} \notin \mathbb{R}$. Considering the u_1-th row of the eigenvalue equation $\lambda(\alpha^\circ) f^\circ = T(\alpha^\circ) f^\circ$, we find

$$0 = \lambda(\alpha^\circ) f_{u_1}^\circ = T(\alpha^\circ)_{u_1,v_1} f_{v_1}^\circ + \sum_{v \neq v_1} T(\alpha^\circ)_{u_1,v} f_v^\circ.$$

Since f° is real and $f_{v_1}^\circ \neq 0$, this implies $T(\alpha^\circ)_{u_1,v}$ is non-real for some $v \neq v_1$. This means that there exists another crossing edge, say the $j = 2$ edge (u_2, v_2), such that $u_1 = u_2$. Then $f_{u_2}^\circ = f_{u_1}^\circ = 0$, so (2.14) implies that the second column of B is zero except for the u_1 component, hence the first and second columns of B are linearly dependent. By Remark 3.4, this implies $\mathrm{rk}(P) > \mathrm{rk}(BPB^*)$, and hence $i_0(\Omega) - i_\infty(S) \geq 1$, which completes the proof. □

We now discuss what the two conditions, $\operatorname{Re} W \geq 0$ and $\det W = 0$, can tell us about the positivity of the matrix W in dimensions $d \leq 3$. In dimension $d = 1$ we immediately get $W = 0$, hence, by Theorem 3.9, any non-corner extremum $\lambda(\alpha^\circ)$ is both a global minimum and a global maximum of $\lambda(\alpha)$. Therefore, $\lambda(\alpha)$ is a "flat band," in agreement with the results of [EKW10]. In dimensions $d = 2, 3$ we have the following results.

Lemma 4.6. *Let W be a 2×2 Hermitian matrix with $\det W = 0$. If $\operatorname{Re} W \geq 0$, then $W \geq 0$.*

Proof. If w is the (potentially) non-zero eigenvalue of W, we have

$$w = \operatorname{tr} W = \operatorname{tr} \operatorname{Re} W \geq 0,$$

and therefore $W \geq 0$. □

Lemma 4.7. *Let W be a 3×3 Hermitian matrix with $\det W = 0$. If $\operatorname{Re} W > 0$, then $W \geq 0$.*

Proof. For convenience we write $W = A + iB$, where A and B are real matrices with $B^T = -B$. The imaginary part iB is a Hermitian matrix with zero trace and determinant. If $B \neq 0$, then $i_+(iB) = i_-(iB) = i_0(iB) = 1$. Since $A > 0$, the Weyl inequalities (for W, as a perturbation of A by iB) yield

$$0 < \lambda_1(A) \leq \lambda_2(W) \leq \lambda_3(W),$$

forcing $\lambda_1(W) = 0$ and therefore $W \geq 0$. □

Theorem 1.3 now follows as a consequence of Theorems 1.2, 2.4 and 4.4, and Lemmas 4.1, 4.6 and 4.7.

Remark 4.8. The strict inequality $\operatorname{Re} W > 0$ in Lemma 4.7 is necessary when $d = 3$. To see this, consider

$$W = \begin{bmatrix} \epsilon & i & 0 \\ -i & \epsilon & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

for any $\epsilon \in (0, 1)$. The matrix W has eigenvalues $-1+\epsilon, 0, 1+\epsilon$, whereas $\operatorname{Re} W$ has eigenvalues $0, \epsilon, \epsilon$. That is, $\det W = 0$ and $\operatorname{Re} W \geq 0$, but W is not non-negative.

When $d = 4$, even strict positivity of $\operatorname{Re} W$ is not enough to guarantee $W \geq 0$. This is illustrated in the example of Section 5.2.2 below.

5. Examples

We present here some illustrative graphs that highlight features of our results, particularly regarding vanishing components of the eigenvector and conjectured necessity of the criterion in Theorem 1.2 (Section 5.1). We also demonstrate that the restrictions on the number of crossing edges, or, in the case of Theorem 1.3(3), on the dimension $d \leq 3$, cannot be dropped without imposing further conditions (Section 5.2).

5.1. **Eigenvectors with vanishing components (Illustration of Theorem 4.4).** A significant effort in the course of the proofs of Section 3 was devoted to treating eigenvectors with some zero components. We were motivated in this effort by some well-known examples that we discuss in Sections 5.1.1 and 5.1.2. In particular, we demonstrate the use of the generalized Haynsworth formula (3.11), needed here because Ω is not invertible. In Section 5.1.3 we revisit the example of [HKSW07] and modify it to test our conjecture that the condition in Theorem 1.2 is not only sufficient but also necessary for the global extremum.

5.1.1. *Honeycomb lattice.* We consider the honeycomb lattice as shown in Figure 1(a) whose fundamental domain consists of two vertices, denoted $\tilde{A}$ and $\tilde{B}$. The tight-binding model on this lattice was used to study graphite [Wal47] and graphene [CNGP$^+$09, Kat12]. For some discussions of the influence of symmetry on the spectrum of this well studied model, see for instance [FW12, BC18]. We have

$$T(\alpha) = \begin{bmatrix} q_{\tilde{A}} & -1 - e^{i\alpha_1} - e^{i\alpha_2} \\ -1 - e^{-i\alpha_1} - e^{-i\alpha_2} & q_{\tilde{B}} \end{bmatrix}, \tag{5.1}$$

where $q_{\tilde{A}}, q_{\tilde{B}}$ are the on-site energies for each sub-lattice. There is an interior global maximum of the bottom band, and an interior global minimum of the top band, at

$$\alpha^\circ = \left(\frac{2\pi}{3}, -\frac{2\pi}{3}\right),$$

as well as their symmetric copies at $-\alpha^\circ$. The eigenvalues are simple unless $q_{\tilde{A}} = q_{\tilde{B}}$ in which case the so-called Dirac conical singularity is formed.

Assume without loss of generality that $q_{\tilde{A}} < q_{\tilde{B}}$ and consider $\lambda = \lambda_1\big(T(\alpha)\big)$. We have

$$\lambda(\alpha^\circ) = q_{\tilde{A}}, \qquad f^\circ = \begin{pmatrix} 1 \\ 0 \end{pmatrix},$$

and

$$T(\alpha^\circ) - \lambda(\alpha^\circ) = \begin{bmatrix} 0 & 0 \\ 0 & q_{\tilde{B}} - q_{\tilde{A}} \end{bmatrix}, \qquad (T(\alpha^\circ) - \lambda(\alpha^\circ))^+ = \begin{bmatrix} 0 & 0 \\ 0 & (q_{\tilde{B}} - q_{\tilde{A}})^{-1} \end{bmatrix}.$$

The derivative matrices B and Ω are

$$B = \begin{bmatrix} 0 & 0 \\ ie^{-i\frac{2\pi}{3}} & ie^{i\frac{2\pi}{3}} \end{bmatrix} \quad \text{and} \quad \Omega = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}.$$

As a result,

$$W = -\frac{1}{q_{\tilde{B}} - q_{\tilde{A}}} \begin{bmatrix} 1 & e^{-i\frac{2\pi}{3}} \\ e^{i\frac{2\pi}{3}} & 1 \end{bmatrix}$$

and $\det(W) = 0$ (in agreement with Theorem 4.4) and $W \leq 0$ (in agreement with $\lambda(\cdot)$ having the global maximum at α°). We also observe that

$$BPB^* = \begin{bmatrix} 0 & 0 \\ 0 & 2 \end{bmatrix},$$

giving $\dim \mathcal{Q} = 1$,

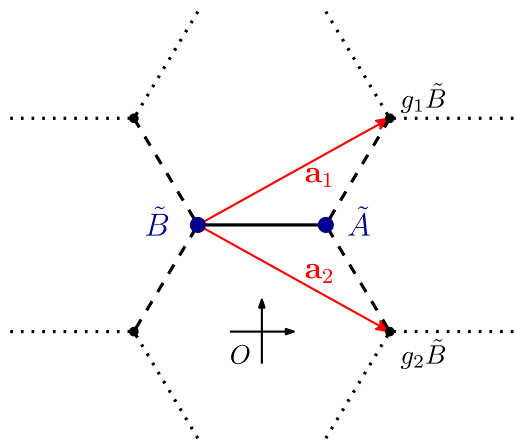
$$S = \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 \\ 0 & q_{\tilde{B}} - q_{\tilde{A}} \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = 0.$$

and $i_\infty(S) = 1$.

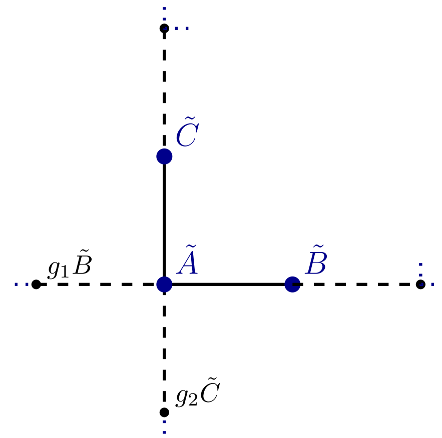
To illustrate Lemma 3.1, we now have, with $A = T(\alpha^\circ) - \lambda(\alpha^\circ)$,

$$\begin{aligned} 1 = i_-(W) &= i_-(\Omega) + i_-(S) + i_\infty(S) - i_-(A) = 0 + 0 + 1 - 0, \\ 1 = i_0(W) &= i_0(\Omega) + i_0(S) - i_\infty(S) - i_0(A) = 2 + 1 - 1 - 1, \\ 0 = i_+(W) &= i_+(\Omega) - i_-(S) - i_0(S) + i_-(A) + i_0(A) = 0 - 0 - 1 + 0 + 1. \end{aligned}$$

We also use this example to demonstrate one of the standard geometric embeddings of the graph. Here we follow the conventions of [CNGP$^+$09, FW12, BC18]. A slightly different (but unitarily equivalent) parameterization is traditionally used in optical lattice studies,



(a)



(b)

FIGURE 4. (a) Fundamental domain of the geometric embedding of honeycomb lattice resulting in Floquet–Bloch representation (5.3); (b) Fundamental domain of the Lieb lattice.

see for instance [Hal88, OPA$^+$19] and related references, though we note here that the latter models often include next-to-nearest neighbors or further connections which are not covered by our results.

The triangle Bravais lattice is the set of points $\Lambda = \{n_1\mathbf{a}_1 + n_2\mathbf{a}_2 \colon (n_1, n_2) \in \mathbb{Z}^2\}$, where the vectors

$$\mathbf{a}_1 = \begin{pmatrix} \sqrt{3}/2 \\ 1/2 \end{pmatrix}, \quad \mathbf{a}_2 = \begin{pmatrix} \sqrt{3}/2 \\ -1/2 \end{pmatrix} \tag{5.2}$$

represent the periodicity group generators g_1 and g_2. Vertices $\tilde{A}$ are placed at locations $\left(\frac{1}{2\sqrt{3}}, \frac{1}{2}\right)^T + \Lambda$, while vertices $\tilde{B}$ are placed at $\left(-\frac{1}{2\sqrt{3}}, \frac{1}{2}\right)^T + \Lambda$, see Figure 4. This way the geometric graph is invariant under rotation by $2\pi/3$ while the reflection $x \mapsto -x$ maps vertices $\tilde{A}$ to $\tilde{B}$ and vice versa.

The reciprocal (dual) lattice, Λ^*, consists of the set of vectors, ξ, such that $e^{\imath v \cdot \xi} = 1$ for every $v \in \Lambda$. The "first Brillouin zone" $\mathcal{B}$, a particular choice of the fundamental domain in the dual space, is defined as the Voronoi cell of the origin in the dual lattice. In this case it is hexagonal.

The Floquet–Bloch transformed operator parametrized by $\mathbf{k} \in \mathcal{B}$ takes the form

$$T(\mathbf{k}) = \begin{bmatrix} q_{\tilde{A}} & -1 - e^{i\mathbf{k}\cdot\mathbf{a}_1} - e^{i\mathbf{k}\cdot\mathbf{a}_2} \\ -1 - e^{-i\mathbf{k}\cdot\mathbf{a}_1} - e^{-i\mathbf{k}\cdot\mathbf{a}_2} & q_{\tilde{B}} \end{bmatrix}. \tag{5.3}$$

While it does not admit a decomposition of the form (2.12), it is related to $T(\alpha)$ of (5.1) by a linear change of variables and so, by Remark 2.3 and Lemma 2.5, we can apply our theorems to the operator (5.3) by directly computing the relevant derivatives in W with respect to the variable $\mathbf{k}$. For the readers convenience, we display the dispersion surfaces on the left of Figure 5.

5.1.2. *Lieb lattice.* As another key example of a model that fits into Theorem 1.3, we consider a version of the Lieb Lattice graph seen in Figure 1(b), consisting of three copies of the square lattice as in Figure 4(b), with $q_{\tilde{A}}, q_{\tilde{B}}, q_{\tilde{C}}$ denoting the on-site energies for each sub-lattice

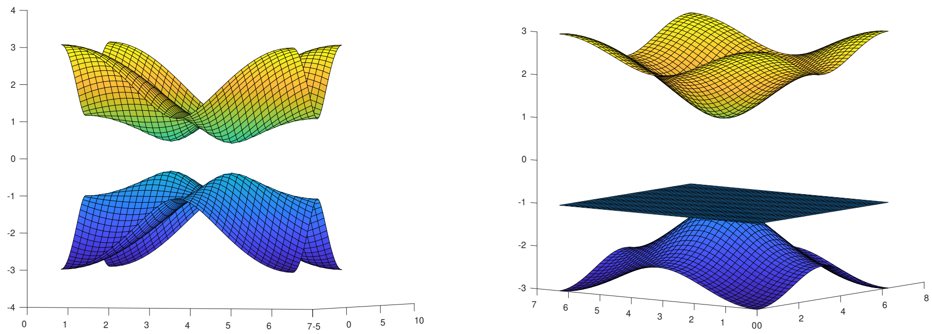


FIGURE 5. The dispersion surfaces of (5.3) (left) and (5.4) (right).

[GSMCB+14, MROB19, MSC+15, SSWX10]. The Floquet–Bloch transformed operator is given by

$$T(\alpha) = \begin{bmatrix} q_{\tilde{A}} & -1-e^{i\alpha_1} & -1-e^{i\alpha_2} \\ -1-e^{-i\alpha_1} & q_{\tilde{B}} & 0 \\ -1-e^{-i\alpha_2} & 0 & q_{\tilde{C}} \end{bmatrix}. \tag{5.4}$$

Taking $q_{\tilde{A}} = 1$ and $q_{\tilde{B}} = q_{\tilde{C}} = -1$, this has eigenvalues

$$\lambda_1(\alpha) = -\sqrt{5 + 2\cos(\alpha_1) + 2\cos(\alpha_2)}, \qquad \lambda_2(\alpha) = -1,$$
$$\lambda_3(\alpha) = \sqrt{5 + 2\cos(\alpha_1) + 2\cos(\alpha_2)}.$$

For the readers convenience, we display the dispersion surfaces on the right in Figure 5. In particular, $\lambda_3(\alpha)$ has a minimum at $\alpha^\circ = (\pi, \pi)$, namely $\lambda_3(\alpha^\circ) = 1$, with an eigenvector $f^\circ = (1, 0, 0)^T$ that vanishes on exactly one end of each crossing edge. We have

$$\Omega = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} = \Omega^+, \qquad B = D\big(T(\alpha)f^\circ\big)\Big|_{\alpha=(\pi,\pi)} = \begin{bmatrix} 0 & 0 \\ -i & 0 \\ 0 & -i \end{bmatrix}$$

and therefore

$$T(\pi,\pi) - \lambda^\circ - B\Omega^+B^* = \begin{bmatrix} 0 & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & -2 \end{bmatrix}, \quad \text{and} \quad BPB^* = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

giving that $\dim \mathcal{Q} = 1$. Then,

$$S = \begin{bmatrix} 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & -2 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} = 0,$$

and $i_\infty(S) = 2$. We also compute

$$W = \Omega - B^*A^+B = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{bmatrix}.$$

We note that because $\alpha = (\pi, \pi)$ is a corner point, Theorem 4.4 ($\det W = 0$) does not apply, but Lemma 4.1 (W is real) does.

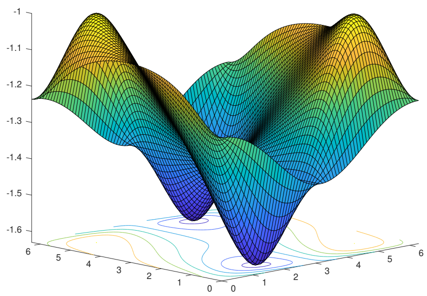


FIGURE 6. The second dispersion surface of (5.5) with $\beta = 0$ (left) and with $\beta = 0.1$ (right).

5.1.3. *A magnetic modification of the example of* [HKSW07]. To give an illustration of Theorem 1.2 with complex H, we modify the example in Figure 2 by adding a magnetic field. Consider the Floquet–Bloch operator

$$T_\beta(\alpha) = \begin{bmatrix} 0 & 0 & e^{i\alpha_1} & 1 & 1+i\beta \\ 0 & 0 & 1 & e^{i\alpha_2} & 1 \\ e^{-i\alpha_1} & 1 & 0 & 1 & 0 \\ 1 & e^{-i\alpha_2} & 1 & 0 & 1 \\ 1-i\beta & 1 & 0 & 1 & 0 \end{bmatrix}, \tag{5.5}$$

which, with $\beta = 0$, reproduces the example considered in [HKSW07]. It was observed in [HKSW07] that the second dispersion band has two maxima at interior points, related by the symmetry $\alpha \mapsto -\alpha$ in the Brillouin zone, see Figure 6(left). Similarly, there are two internal minima. Non-zero β adds a slight magnetic field term on the $1 \to 5$ edge of the form and breaks the symmetry in the dispersion relation. One maximum becomes larger (and hence the global maximum) and the other one smaller (merely a local maximum), as can be seen in Figure 6(right).

Taking $\beta = 0.1$, the locations of the two maxima of $\lambda_2\big(T_\beta(\alpha)\big)$ were numerically computed using *Matlab* (both using an optimization solver `fminunc` and a root finder `fsolve`) to be at $(\alpha_1^g, \alpha_2^g) \approx (1.0632, 5.2200)$ and $(\alpha_1^\ell, \alpha_2^\ell) \approx (5.2534, 1.0298)$. Computing their corresponding eigenvectors f° and using equation (2.8) the gradient was verified to be zero with error of less than 4×10^{-16} for both critical points. For this model, following Lemmas 2.6 and 2.7 we have

$$\Omega = \begin{bmatrix} -\operatorname{Re}(e^{i\alpha_1^\circ} f_3^\circ \overline{f_1^\circ}) & 0 \\ 0 & -\operatorname{Re}(e^{i\alpha_2^\circ} f_4^\circ \overline{f_2^\circ}) \end{bmatrix}, \qquad B = \begin{bmatrix} ie^{i\alpha_1^\circ} f_3^\circ & 0 \\ 0 & ie^{i\alpha_2^\circ} f_4^\circ \\ -ie^{-i\alpha_1^\circ} f_1^\circ & 0 \\ 0 & -ie^{-i\alpha_2^\circ} f_2^\circ \\ 0 & 0 \end{bmatrix} \tag{5.6}$$

and as a result we can easily compute the eigenvalues of $W = \Omega - B^*(T(\alpha^\circ) - \lambda_2 I)^+ B$. At the global maximum, W is found to have two negative eigenvalues, $\{-0.3433, -0.0095\}$, whereas at the local maximum W is sign-indefinite with eigenvalues $\{-0.3240, 0.0097\}$, the signs of which are determined up to errors much larger than those in our calculations. Analogous results hold for the global and local minima.

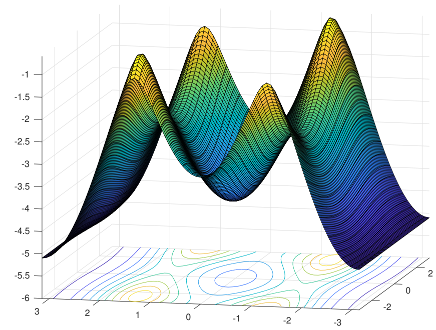


FIGURE 7. An example of a dispersion band on a $\mathbb{Z}^2$-periodic graph Γ with a local (but not global) minimum resulting from multiple edges per generator.

This example motivates the following.

Conjecture. *Under the assumptions of Theorem 1.2, a critical point α° is a global minimum if and only if $W \geq 0$, and a global maximum if and only if $W \leq 0$.*

5.2. **(Counter)-examples.** In this section we provide examples showing that the assumptions in our theorems are necessary. First, in Section 5.2.1, we show that the assumption in Theorems 1.2 and 1.3 that the graph has one crossing edge per generator is needed. Next, in Section 5.2.2 we show that, even when H is real-symmetric, the conclusion of Theorem 1.3 fails for $d = 4$.

The example in Section 5.2.1 demonstrates one of the simplest possible ways of adding multiple edges per generator in the context of a 2×2 model $T(\alpha)$, but the form of the operator was motivated by the Haldane model [Hal88], which includes next nearest neighbor complex hopping terms in the form of $T(k)$ given in (5.3). We observe by directly computing the eigenvalues that the dispersion relation can have a local minimum that is not a global minimum.

5.2.1. *Multiple edges per generator.* To see that the condition on one edge per generator is required, we first consider a model similar to that of the Honeycomb lattice, but with another edge for one of the generators, specifically given by

$$T(\alpha) = \begin{bmatrix} -1 + t\cos(\alpha_2) & -1 - e^{i\alpha_1} - e^{i\alpha_2} \\ -1 - e^{-i\alpha_1} - e^{-i\alpha_2} & 1 - t\cos(\alpha_2) \end{bmatrix},$$

where we have introduced multiple edges per generator and for simplicity chosen $q_{\tilde{A}} = -1$ and $q_{\tilde{B}} = 1$. For t sufficiently large, we observe that the branch for $\lambda_1(\alpha)$ has a local minimum that is not a global minimum, as shown in the dispersion surface plotted in Figure 7, where we have taken $t = 4$ and thus the lowest dispersion surface is described by the function

$$\lambda_1(\alpha) = -\sqrt{2(6 + \cos(\alpha_1) + \cos(\alpha_1 - \alpha_2) - 3\cos(\alpha_2) + 4\cos(2\alpha_2))}.$$

The local minimum here occurs at $\alpha = (0, 0)$, which is a corner point and hence we have that $W = \operatorname{Re} W$ and the local minimum will have a positive definite quadratic form. Hence, we can observe this as a counterexample to both Theorems 1.2 and 1.3 in the case of multiple edges per generator.

Our example in this section was motivated by the Haldane model, which is $\mathbb{Z}^2$-periodic. However, even $\mathbb{Z}^1$-periodic graph operators are not immune from this problem, see [EKW10] and [Shi14, Example 1].

5.2.2. *Dimension* $d \geq 4$. We construct here a random graph with $\mathbb{Z}^4$ symmetry that displays a local extremum that is not a global extremum. The example was found by searching through positive rank-one perturbations of a random symmetric matrix having 1 as a degenerate eigenvalue; this insured that 1 is a local (but not necesarily global) maximum. As a trigger for terminating the search we used the conjecture in Section 5.1.3: the matrix W was computed and the search was stopped when it was sign-indefinite. The resulting example revealed the presence of a global maximum elsewhere, thus also serving as a numerical confirmation of the conjecture's veracity. We report it with all entries rounded off for compactness.

$$T(\alpha) =$$
$$\begin{bmatrix} 2.556782 & .104696 & -.000742 & -.049562 & -.072260 \\ .104696 & 3.69455 & -.436154 & -.126495 & -.571811 \\ -.000742 & -.4361543 & 15.033535 & .139015 & -.363838 \\ -.049562 & -.126495 & .139015 & 2.146425 & .298246 \\ -.072260 & -.571811 & -.363838 & .298246 & 9.097398 \end{bmatrix} + \begin{bmatrix} 0 & e^{i\alpha_1} & e^{i\alpha_2} & -e^{i\alpha_3} & e^{i\alpha_4} \\ e^{-i\alpha_1} & 0 & 0 & 0 & 0 \\ e^{-i\alpha_2} & 0 & 0 & 0 & 0 \\ -e^{-i\alpha_3} & 0 & 0 & 0 & 0 \\ e^{-i\alpha_4} & 0 & 0 & 0 & 0 \end{bmatrix}.$$

Using the objective function of the form $\lambda_1\big(T(\alpha)\big)$ and running a Newton BFGS optimization with randomly seeded values of α, we find two distinct local maxima at $\alpha^\circ \approx (-1.488, -2.153, 1.553, -3.324)$ and $\lambda_1(\alpha^\circ) \approx 0.989459$ (close but not equal to 1 due to rounding off the entries of the example matrix). However, the observed global maximum is $\lambda_1(\pi, 0, \pi, 0) \approx 1.2467$. Hence, we observe that the corner point is a local maximum that is in fact a global maximum (as follows from Theorem 1.3(1)), but the interior point is a local maximum that is not a global maximum. The minimum of the second band appears to be 2.63496, hence there are no degeneracies arising between the first two spectral bands.

Appendix A. A generalized Haynsworth formula

The inertia of a Hermitian matrix M is defined to be the triple

$$\mathrm{In}(M) = (i_+(M), i_-(M), i_0(M)) \tag{A.1}$$

of numbers of positive, negative and zero eigenvalues of M, respectively. For a Hermitian matrix in block form,

$$M = \begin{pmatrix} A & B \\ B^* & C \end{pmatrix}, \tag{A.2}$$

the Haynsworth formula [Hay68] shows that, if A is invertible, then

$$\mathrm{In}(M) = \mathrm{In}(A) + \mathrm{In}(M/A), \tag{A.3}$$

where

$$M/A := C - B^*A^{-1}B \tag{A.4}$$

is the Schur complement of the block A. We are concerned with the case when the matrix A is singular. In this case, inequalities extending (A.3) have been obtained by Carlson et al. [CHM74] and a complete formula was derived by Maddocks [Mad88, Thm 6.1]. Here we propose a different variant of Maddocks' formula. Our variant makes the correction terms more transparent and easier to calculate; they are motivated by a spectral flow picture. They are also curiously similar to the answers obtained in a related question by Morse [Mor71] and Cottle [Cot74].

Theorem A.1. *Suppose M is a Hermitian matrix in the block form* (A.2)*, and let P denote the orthogonal projection onto* $\mathrm{Null}(A)$*. Then*

$$\mathrm{In}(M) = \mathrm{In}(A) + \mathrm{In}_{\mathcal{Q}}(M/A) + (i_\infty, i_\infty, -i_\infty), \tag{A.5}$$

where the subspace $\mathcal{Q}$ is defined by

$$\mathcal{Q} = \mathrm{Null}(B^*PB), \tag{A.6}$$

$\mathrm{In}_{\mathcal{Q}}(X)$ *stands for the inertia of X restricted to the subspace $\mathcal{Q}$, and i_∞ is given by*

$$i_\infty = i_\infty(M/A) = \mathrm{rk}(B^*PB) = \dim(C) - \dim(\mathcal{Q}). \tag{A.7}$$

Remark A.2. If the matrix A is singular, equation (A.4) is not appropriate for defining the Schur complement. It is usual to consider the generalized Schur complement

$$M/A := C - B^*A^+B,$$

where A^+ is the Moore–Penrose pseudoinverse, which is what we have done in the main arguments above. However, because of the restriction to $\mathcal{Q}$, any reasonable generalization will work in equation (A.5). For example,

$$M/A_\epsilon := C - B^*(A + \epsilon P)^{-1}B, \tag{A.8}$$

is well defined for any $\epsilon \neq 0$. Taking the limit $\epsilon \to \infty$, we recover the definition with A^+. In fact, it can be shown that

$$M/A_\epsilon = M/A - \tfrac{1}{\epsilon}B^*PB,$$

with the last summand being identically zero on the subspace $\mathcal{Q}$. It follows that the restriction $(M/A_\epsilon)_{\mathcal{Q}} = (M/A)_{\mathcal{Q}}$ is *independent of* ϵ, so the index $\mathrm{In}_{\mathcal{Q}}(M/A_\epsilon)$ is as well.

Remark A.3. The index $i_\infty(M/A)$ has a beautiful geometrical meaning: it is the number of eigenvalues of M/A_ϵ which escape to infinity as $\epsilon \to 0$. Correspondingly, $\mathrm{In}_Q(M/A)$ counts the eigenvalues of M/A_ϵ converging to positive, negative and zero *finite* limits as $\epsilon \to 0$.

Remark A.4. As a self-adjoint linear relation, the Schur complement M/A is well defined even if A is singular (see, for example, [CdV99]). Then the index $i_\infty(M/A)$ has the meaning of the dimension of the multivalued part whereas $\mathrm{In}_Q(M/A)$ is the inertia of the operator part of the linear relation (see, for example, [Sch12, Sec 14.1] for relevant definitions).

The proof of Theorem A.1 follows simply from the following formula, which was proved in the generality we require in [JMRT87] (inspired by a reduced version appearing in [HF85]). The original proofs are of "linear algebra" type. For geometric intuition we will provide a "spectral flow" argument in Section A.1.

Lemma A.5 (Jongen-Möbert-Rückmann-Tammer, Han-Fujiwara)**.** *The inertia of the Hermitian matrix*

$$M = \begin{pmatrix} 0_m & B \\ B^* & C \end{pmatrix}, \tag{A.9}$$

where 0_m is the $m \times m$ zero matrix, is given by the formula

$$\mathrm{In}(M) = \mathrm{In}_{\mathrm{Null}(B)}(C) + (\mathrm{rk}(B), \mathrm{rk}(B), m - \mathrm{rk}(B)). \tag{A.10}$$

Proof of Theorem A.1. Take A and M as given by (A.2). Let $V = (V_1\ V_0)$ be the unitary matrix of eigenvectors of A, with V_0 being the $m = \dim \mathrm{Null}(A)$ eigenvectors of eigenvalue 0. We have

$$V^* A V = \begin{pmatrix} \Theta & 0 \\ 0 & 0_m \end{pmatrix},$$

where Θ is the non-zero eigenvalue matrix of A and only the most important block size is indicated. We recall that, with the above notation, the Moore–Penrose pseudoinverse is given by $A^+ = V_1 \Theta^{-1} V_1^*$.

Conjugating M by the block-diagonal matrix $\mathrm{diag}(V, I)$, we obtain the unitary equivalence

$$M \simeq \begin{pmatrix} \Theta & 0 & V_1^* B \\ 0 & 0 & V_0^* B \\ B^* V_1 & B^* V_0 & C \end{pmatrix}.$$

Applying the Haynsworth formula to the invertible matrix Θ, we get

$$\mathrm{In}(M) = \mathrm{In}(\Theta) + \mathrm{In} \begin{pmatrix} 0 & V_0^* B \\ B^* V_0 & C - B^* V_1 \Theta^{-1} V_1^* B \end{pmatrix}.$$

We now apply Lemma A.5 to get

$$\mathrm{In}(M) = \mathrm{In}(\Theta) + \mathrm{In}_Q \left(C - B^* V_1 \Theta^{-1} V_1^* B \right) + (i_\infty, i_\infty, m - i_\infty),$$

since $\mathrm{Null}(V_0^* B) = \mathrm{Null}(B^* P B) = \mathcal{Q}$ and $\mathrm{rk}(V_0^* B) = \mathrm{rk}(B^* P B) = i_\infty$. We finish the proof by observing that $\mathrm{In}(\Theta) + (0, 0, m) = \mathrm{In}(A)$ and $C - B^* V_1 \Theta^{-1} V_1^* B$ is equal to the generalized Schur complement $C - B^* A^+ B = M/A$. □

A.1. **An alternative proof of Lemma A.5.** To give a perturbation theory intuition behind Lemma A.5, define

$$M_\epsilon = \begin{pmatrix} \epsilon I_m & B \\ B^* & C \end{pmatrix}. \tag{A.11}$$

For $\epsilon > 0$, M_ϵ is a non-negative perturbation of M. When ϵ is small enough, none of the negative eigenvalues of M will cross 0, therefore $i_-(M_\epsilon) = i_-(M)$. Applying the Haynsworth formula to the invertible matrix ϵI, we get

$$i_-(M) = i_-(M_\epsilon) = i_-(\epsilon I) + i_- \left(C - \tfrac{1}{\epsilon} B^* B \right) = i_- \left(C - \tfrac{1}{\epsilon} B^* B \right).$$

Due to the presence of $\frac{1}{\epsilon}$, some eigenvalue of $M/\epsilon := C - \frac{1}{\epsilon} B^* B$ becomes unbounded. More precisely, the Hilbert space on which C is acting can be decomposed as

$$H_C = \mathrm{Ran}(B^* B) \oplus \mathrm{Null}(B^* B). \tag{A.12}$$

There are $\mathrm{rk}(B^* B)$ eigenvalues of M/ϵ going to $-\infty$ as $\epsilon \to 0$. The rest of the eigenvalues of M/ϵ converge to eigenvalues of C restricted to $\mathrm{Null}(B^* B)$. Informally, the operator M/ϵ is reduced by the above Hilbert space decomposition in the limit $\epsilon \to 0$. This argument can be made precise by applying the Haynsworth formula to M/ϵ written out in the block form in the decomposition (A.12).

The negative eigenvalues of $i_-(M_\epsilon)$ thus come from $\mathrm{rk}(B^* B) = \mathrm{rk}(B)$ eigenvalues going to $-\infty$, and the negative eigenvalues of C on $\mathrm{Null}(B^* B) = \mathrm{Null}(B)$. This establishes the negative index in equation (A.10). Positive eigenvalues are calculated similarly by considering small negative ϵ, and the zero index can be obtained from the total dimension.

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