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TORIC GEOMETRY AND DISCRETE PERIODIC OPERATORS

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Abstract. This is an extended version of an Oberwolfach report accompanying a talk by Sottile in March 2022, and may serve as an introduction for algebraic geometers to recent work applying methods from algebraic geometry to the study of operators on periodic graphs. It includes more references, background, and a brief discussion of current work.

Introduction

The standard Schrödinger operator (Laplacian plus potential) is fundamental in quantum mechanics. Its spectrum records the energy levels of particles. On a periodic medium, and after Fourier (Floquet) transform, the spectrum becomes an analytic hypersurface in $\mathbb{T}^d \times \mathbb{R}$, revealing more of its structure. Here, $\mathbb{T}$ is the unit circle and d is the ambient dimension. Discretizing gives an operator on a (weighted) $\mathbb{Z}^d$-periodic graph whose spectrum is an algebraic hypersurface in $\mathbb{T}^d \times \mathbb{R}$. Several physically important properties then become questions in algebraic geometry, including the nondegeneracy of spectral edges, embedded eigenvalues, and the density of states.

Some of these questions were spectacularly addressed in the 1990's in papers by Bättig, Gieseker, Knörrer, and Trubowicz. This was for a particular periodic graph (the grid graph), using a compactification in a toroidal embedding. The ensuing 30 years have seen a deepening of the theory of toric varieties along with a development of spectral theory (and more open questions). This document (based on a talk at Oberwolfach in March 2022) sketches some of this story, in particular that these questions remain open for operators on more general discrete periodic graphs. It may serve as an informal introduction to this emerging application area.

1. Bloch Varieties of Discrete Periodic Operators

For background, see [1, 17, 18, 25]. A recent paper discussing the algebraic persepctive is [7]. A fundamental problem in mathematical physics is to understand the spectrum $\sigma(L)$ of a Schrödinger operator L acting on complex-valued functions on $\mathbb{R}^d$. For such a function f, we have

$$Lf \;=\; L(f) \;:=\; -\Delta f \;+\; Vf\,,$$

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where $\Delta = \sum_i \frac{\partial^2}{\partial x_i^2}$ is the Laplacian operator and $V\colon \mathbb{R}^d \to \mathbb{R}$ is a potential function. As L is a self-adjoint operator on an appropriate Hilbert space, its spectrum is a closed subset of $\mathbb{R}$.

Solid-state physics compels us to consider the Schrödinger operator in a crystalline material, where the Laplacian may be altered to reflect a periodic anisotropy and the potential V is a periodic function. That is, we have an action of $\mathbb{Z}^d$ on $\mathbb{R}^d$ by translation such that for $x \in \mathbb{R}^d$ and $\gamma \in \mathbb{Z}^d$, $V(\gamma{+}x) = V(x)$, and the Laplacian is replaced by a ($\mathbb{Z}^d$-periodic) Laplace-Beltrami operator $\sum_{i,j} c_{i,j} \frac{\partial^2}{\partial x_i \partial x_j}$. In this setting, the spectrum of the Schrödinger operator consists of a union of intervals in $\mathbb{R}$, giving the familiar structures of spectral bands and spectral gaps.

Consider the following very general discrete version of this problem. Let Γ be a graph equipped with a free action of $\mathbb{Z}^d$ having finitely many orbits on its edges, $\mathcal{E}(\Gamma)$, and vertices, $\mathcal{V}(\Gamma)$. Fix parameters, functions $c\colon \mathcal{E}(\Gamma) \to \mathbb{R}$ and $V\colon \mathcal{V}(\Gamma) \to \mathbb{R}$ that are $\mathbb{Z}^d$-periodic. The Schrödinger operator L acts on a complex-valued function $f\colon \mathcal{V}(\Gamma) \to \mathbb{C}$, as

$$Lf(v) \ :=\ V(v)f(v) \ +\ \sum_{u\sim v} c_{(u,v)}(f(v) - f(u))\,.$$

Here, $u \sim v$ indicates that u and v are connected by an edge, (u,v). When $c_{(u,v)} = 1$ is constant, the sum is the graph Laplacian and general parameters model a periodic anisotropy or interaction strength along edges so that the sum becomes a discrete Laplace-Beltrami operator. Then L is an operator on $\ell^2(\Gamma)$, the space of square-summable functions on $\mathcal{V}(\Gamma)$.

Fourier transform (typically called Floquet transform in the literature) reveals more structure of the spectrum $\sigma(L)$. Let $\mathbb{T} \subset \mathbb{C}$ be the unit complex numbers. For $x \in \mathbb{T}$, $\overline{x} = x^{-1}$. Then $\mathbb{T}^d := \operatorname{Hom}(\mathbb{Z}^d, \mathbb{T})$ is the space of unitary characters of $\mathbb{Z}^d$. The evaluation of $z \in \mathbb{T}^d$ at $\gamma \in \mathbb{Z}^d$ is a monomial, $z(\gamma) = z_1^{\gamma_1} \cdots z_d^{\gamma_d} =: z^\gamma$, which we view as a function on $\mathbb{T}^d$. The Fourier transform of a function $f(v)$ on $\mathcal{V}(\Gamma)$ is a function $\hat{f}(z,v)$ on $\mathbb{T}^d \times \mathcal{V}(\Gamma)$ that is quasi-periodic in that $\hat{f}(z, \gamma + v) = z^\gamma \hat{f}(z,v)$. If we let W be a fundamental domain for the action of $\mathbb{Z}^d$ on $\mathcal{V}(\Gamma)$, then Fourier transform is a linear isometry between $\ell^2(\Gamma)$ and $L^2(\mathbb{T}^d)^W$, the space of functions $\hat{f}\colon W \to L^2(\mathbb{T}^d)$. The action of the operator L on such functions $\hat{f}$ becomes

$$L\hat{f}(v) \ :=\ V(v)\hat{f}(v) \ +\ \sum_{\gamma+u\sim v} c_{(\gamma+u,v)}(\hat{f}(v) - z^\gamma \hat{f}(u))\,. \tag{1}$$

Example 1. On the left in Figure 1 is the crystalline structure of graphene, called the honeycomb lattice. a $\mathbb{Z}^2$-periodic graph. Its fundamental domain W has two vertices u and v, and there are three orbits of edges. Fix edge parameters p, q, r, as on the right. The operator L is

$$\begin{aligned}
L\hat{f}(u) &= V(u)\hat{f}(u) + p(\hat{f}(u) - \hat{f}(v)) + q(\hat{f}(u) - x^{-1}\hat{f}(v)) + r(\hat{f}(u) - y^{-1}\hat{f}(v))\ ,\\
L\hat{f}(v) &= V(v)\hat{f}(v) + p(\hat{f}(v) - \hat{f}(u)) + q(\hat{f}(v) - x\hat{f}(u)) \quad + r(\hat{f}(v) - y\hat{f}(u))\ .
\end{aligned}$$

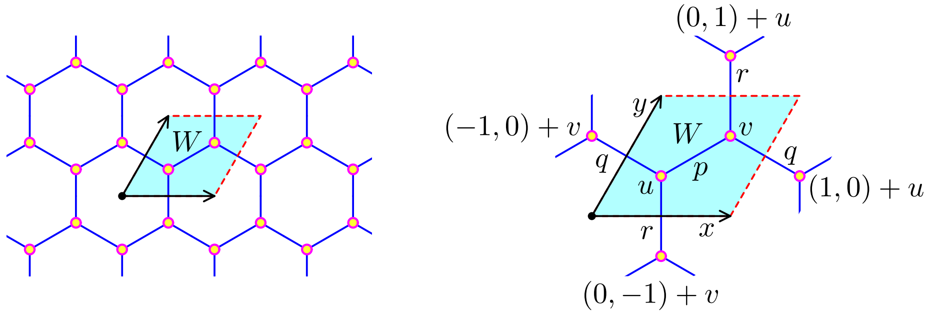

FIGURE 1. Honeycomb lattice and $\mathbb{Z}^2$-periodic edge parameters.

Collecting coefficients of $\hat{f}(u), \hat{f}(v)$, we may represent L by the 2×2-matrix,

$$L \;=\; \begin{pmatrix} V(u)+p+q+r & -p-qx^{-1}-ry^{-1} \\ -p-qx-ry & V(v)+p+q+r \end{pmatrix} ,$$

whose entries are Laurent polynomials in x, y. Observe that for $(x,y)\in\mathbb{T}^2$, $L^T=\overline{L}$, so that L is Hermitian and thus the operator L is self-adjoint.

What we saw in Example 1 holds in general. After Fourier transform, the operator L is multiplication by a $W\times W$ matrix $L(z)$ of Laurent polynomials in $z\in\mathbb{T}^d$. As Γ is an undirected graph, $L^T(z)=L(z^{-1})$, and thus $L^T(z)=\overline{L(z)}=L(\overline{z})$, as $z\in\mathbb{T}^d$. In particular, for $z\in\mathbb{T}^d$, $L(z)$ is Hermitian and hence has $|W|$ real eigenvalues. As $z\in\mathbb{T}^d$ varies, these real eigenvalues determine $|W|$ band functions over $\mathbb{T}^d$.

There is another, global perspective on the band functions. These eigenvalues are the roots of the characteristic polynomial $D(z,\lambda)=\det(L(z)-\lambda I)$. Viewed as a polynomial in z,λ, it is the dispersion polynomial which defines the Bloch variety, $\{(z,\lambda)\mid D(z,\lambda)=0\}$, a hypersurface in $\mathbb{T}^d\times\mathbb{R}$. The Bloch variety is the union of the graphs of the spectral band functions. Figure 2 shows two Bloch varieties for the honeycomb lattice with zero potential. On the left the edge parameters are 6, 3, 2, and on the right they are 1, 1, 1, giving the graph Laplacian. The spectrum $\sigma(L)$ of the original operator L is the image of the Bloch variety

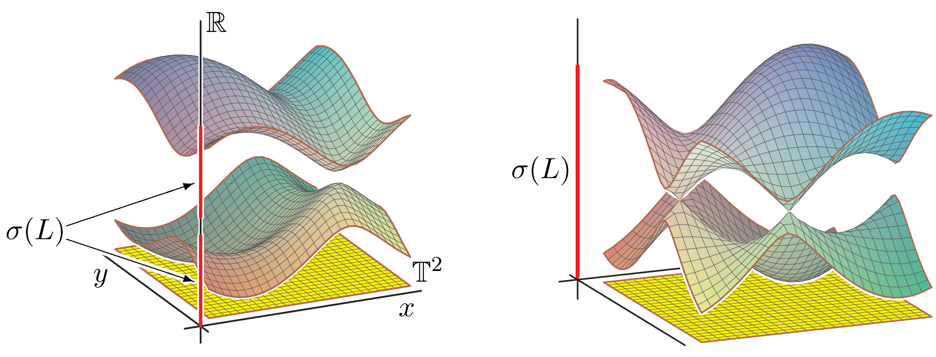

FIGURE 2. Bloch varieties with edge parameters 6,3,2 and 1,1,1.

under projection to the vertical λ-axis. The Bloch variety on the left has two spectral bands with a gap in between, while the Bloch variety for the Laplacian on the right, there is one spectral band. The singularities joining the two sheets are conical ordinary double points, called Dirac points in the literature. We also consider Fermi varieties, which are identified with level sets of the coordinate λ on a Bloch variety.

Since Bloch and Fermi varieties are defined by Laurent polynomials $D(x,\lambda)$, it is natural to complexify, allowing the parameters c and V to be complex-valued, $z\in(\mathbb{C}^\times)^d$, and $\lambda\in\mathbb{C}$. This gives complex Bloch and Fermi varieties, which are hypersurfaces in $(\mathbb{C}^\times)^d\times\mathbb{C}$ and $(\mathbb{C}^\times)^d$, respectively. The complex Bloch variety is viewed in this subject as the graph of a multi-valued extension $\lambda\colon(\mathbb{C}^\times)^d\to\mathbb{C}_\lambda$ of the band functions. We adopt the geometric perspeective that λ i=s (a coordinate) coordinate function on the Bloch Variety.

This illuminates the original real Bloch and Fermi varieties, showing that they are real algebraic varieties. Indeed, the map $(z,\lambda)\mapsto(\overline{z^{-1}},\overline{\lambda})$ is an antiholomorphic involution on $(\mathbb{C}^\times)^d\times\mathbb{C}$, and thus endows $(\mathbb{C}^\times)^d\times\mathbb{C}$ with the structure of a real algebraic variety, which is not its standard real structure. When the parameters c and V are real, the identity $L^T(z)=L(z^{-1})$ implies that the dispersion polynomial $D(z,\lambda)=\det(L(z)-\lambda I)$ is fixed by this involution. Consequently, the complex Bloch variety is stable under this involution, which gives it a (non-standard) structure as a real algebraic variety, with the real Bloch variety its set of real points. The same is true for the complex and real Fermi varieties, when λ is real.

There are several fundamental questions from physics which may be understood in terms of the geometry of these objects. The spectral edges conjecture posits that for L sufficiently general (e.g. c,V general), the extrema of the function λ on the real Bloch variety are nondegenerate. Generality is impostant as the example of Filonov Kachovskiy [13] shows. Here, nondegenerate means that the Hessian of the band function is invertible. This is explicitly stated in [18, Conj. 5.25], and it appears in other sources [5, 17, 22, 23]. Important notions, such as effective masses in solid state physics, the Liouville property, Green's function asymptotics, Anderson localization, homogenization, and many other assumed properties depend upon this conjecture. This is discussed in [7, Sect. 1.4].

This holds for the two Bloch varieties in Figure 2. On the Bloch variety at left, λ is a Morse function, and all critical points are nondegenerate. The critical value from the singularities on the Bloch variety of the Laplacian lies in the interior of the spectrum and the corresponding extrema of the band functions are nondegenerate even though they do not give edges of the spectrum. A first step towards the spectral edges conjecture may be to understand the critical points of λ. This was used in [7] to prove the spectral edges conjecture for the graph on the left of Figure 4. A strengthening of the spectral edges conjecture is the critical points conjecture: For generic parameters, all critical points of λ on the Bloch variety are nondegenerate.

A local perturbation of L may lead to compactly supported states. The eigenvalue (energy) λ of such a state may occur within a spectral band of L (this is the physically undesirable situation of an embedded eigenvalue) only if the complex Fermi variety at λ is reducible [19]. Irreducibility of the Bloch variety is also of interest for then its smooth complex points are path-connected and thus the Bloch variety is determined by the neighborhood of any point.

2. Classical work

Around 1990, Bättig, Gieseker, Knörrer, and Trubowicz [3, 12] settled a number of questions in the following situation. Suppose that Γ is the grid graph, whose vertices are $\mathbb{Z}^d$ with $\alpha, \beta \in \mathbb{Z}^d$ adjacent if $\alpha - \beta \in \{\pm e_1, \ldots, \pm e_d\}$, where $e_1, \ldots, e_d$ are the standard generators of $\mathbb{Z}^d$. If we let e_i act as translation by $a_i e_i$ for a_i a positive integer, then Γ is $\mathbb{Z}^d$-periodic with fundamental domain the integer points in any $a_1 \times \cdots \times a_d$ box. Suppose that $d = 2$, set $a = a_1$ and $b = a_2$, and assume that they are relatively prime.

The Schrödinger operator with the graph Laplacian depends upon ab parameters, the values of the potential V on a fundamental domain. Gieseker, Knörrer, and Trubowicz [12] prove identifiability: if V and V' are general and give the same Bloch variety, then V and V' differ only by obvious symmetries of relabeling the fundamental domain. This was later extended to all d by Kappeler [14].

Also in [12], it is shown that there is a dense open set of $\mathbb{C}^{ab}$ consisting of potentials V such that the function λ on the Bloch variety has exactly

$$2a^2b^2 + 6ab(a + b) + 12ab - 12(a^2 + b^2) - 2(a + b) - 12 \tag{2}$$

critical values. For potentials in this open set, the Bloch variety is smooth and irreducible, all Fermi surfaces are irreducible curves, and are at most nodal. Furthermore, they determine the density of states, e.g. the distribution of the eigenvalues of the Laplacian. Bättig extended some of this to Fermi surfaces when $d = 3$ [3].

These and other results were surveyed in a Bourbaki lecture by Peters [24]. They were obtained by compactifying the Bloch and Fermi varieties in a natural toric variety, followed by a toric resolution of singularities. Another intriguing result is a 'directional compactification' of the Bloch variety in the original, nondiscrete setting when the Bloch variety is an analytic variety and consists of countably many sheets above $\mathbb{T}^3$ [2].

3. Current work

We describe some results obtained with Faust [9]. Consider a Schrödinger operator L on a periodic graph Γ, with fundamental domain $W \subset \mathcal{V}(\Gamma)$ and complex parameters c, V. After Fourier transform, the operator $L = L(z)$ is a $W \times W$ matrix whose row indexed by $v \in W$ is determined by (1), and its entry in position (v, u) is a Laurent polynomial recording the edges in Γ between v and translates $\gamma + u$, with additional constant terms when $v = u$.

The dispersion polynomial $D(z, \lambda) = \det(L(z) - \lambda I)$ is a Laurent polynomial which is an ordinary polynomial in λ that is monic and of degree $|W|$. Let $P_\Gamma \subset \mathbb{R}^{d+1}$ be its Newton polytope—the convex hull of the exponent vectors of all monomials in z, λ occurring in $D(z, \lambda)$. We are suppressing the dependence on the parameters c and V, but there is an open subset of parameters yielding the same polytope, which we write as $\mathcal{N}(\Gamma)$. Figure 3 shows Newton polytopes for the honeycomb graphs and for the two graphs of Figure 4. These are viewed from the positive orthant and λ is the vertical axis.

Let $X^\circ = (\mathbb{C}^\times)^d \times \mathbb{C}$, the domain of the dispersion polynomial $D(z, \lambda)$ and the ambient space of the Bloch variety. This has a natural compactification given by the projective toric variety X_Γ corresponding to the polytope P_Γ, and the closure of the Bloch variety in X_Γ is a compactification of the Bloch variety.

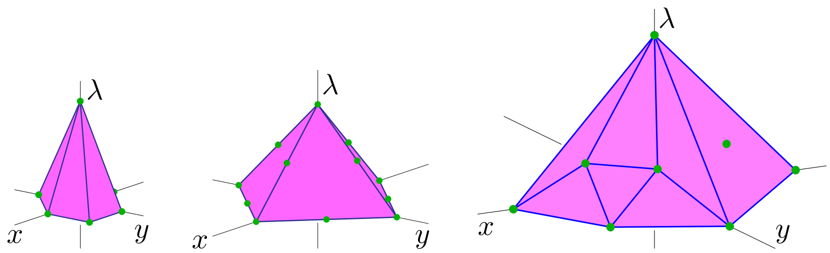

FIGURE 3. Three Newton Polytopes.

The symmetry $L(z)^T = L(z^{-1})$ implies that the Newton polytope $P_\Gamma \subset \mathbb{R}^d \times \mathbb{R}$ is symmetric about the origin in its first d coordinates, $(\alpha, b) \mapsto (-\alpha, b)$, corresponding to exponents of z. The theory of arithmetic toric varieties developed in [8] is relevant to these questions (see also [21]). The toric variety X_Γ has a non-standard real structure extending that of $X^\circ\colon (z,\lambda) \mapsto (\overline{z^{-1}}, \overline{\lambda})$. When the parameters c and V are real, this restricts to the compactified Bloch variety, revealing it to be a real hypersurface in the arithmetic toric variety X_Γ. This explains some aspects of its structure and enables tools from real algebraic geometry to be used to study Bloch varieties.

A main result in [9] is a generalization of the enumeration (2) of critical values in [12]. A critical point of the function λ on the Bloch variety is a point of the Bloch variety where the gradients (in the ambient $(\mathbb{C}^\times)^d$
CC of λ and $D(z,\lambda)$ are linearly dependent. These are singular points of the Bloch variety or points where $\frac{\partial D}{\partial z_i}(z,\lambda) = 0$ for $i = 1, \dots, d$ and $\frac{\partial D}{\partial \lambda}(z,\lambda) \neq 0$. Thus a point $(z,\lambda) \in X^\circ$ is a critical point of the function λ on the Bloch variety if and only if it is a common zero of the polynomials

$$D(z,\lambda)\,,\ z_1\frac{\partial}{\partial z_1}D(z,\lambda)\,,\ \dots\,,\ z_d\frac{\partial}{\partial z_d}D(z,\lambda)\,. \tag{3}$$

(As $z_i \in \mathbb{C}^\times$, it is no harm to multiply $\frac{\partial}{\partial z_i}D(z,\lambda)$ by z_i.)

Observe that each polynomial in (3) has Newton polytope that is a subset of P_Γ. Consequently, the critical points are the common zeroes on X° of $d{+}1$ sections of the line bundle $\mathcal{O}(P_\Gamma)$ on X_Γ. Kushnirenko's Theorem [15] gives the following bound.

Theorem 2. *The number of critical points of the function λ on the Bloch variety is at most the degree of the toric variety X_Γ, which is $(d{+}1)!\mathrm{vol}(P_\Gamma)$.*

An application of Bernstein's Theorem B [4] (or simple projective geometry) informs us that if the number of critical points of λ on the Bloch variety is less than the degree of X_Γ, then the critical point equations (3) have solutions in $\partial X_\Gamma := X_\Gamma \setminus X^\circ$.

By the structure of projective toric varieties [6], we obtain X_Γ from X° by adding divisors for each facet of P_Γ, except its base (as $\lambda = 0$ is a subset of X°). Each face F of P_Γ corresponds to a torus orbit X°_F on X_Γ whose closure is the toric variety corresponding to F. The intersection of X°_F with the compactified Bloch variety is defined by the restriction $D(z,\lambda)|_F$ of $D(z,\lambda)$ to the monomials whose exponent vectors lie in F.

Theorem 3. *If the critical point equations* (3) *have a solution $x_F \in X_F^\circ$, for F a face of P_Γ that is not its base, then either F is vertical or the hypersurface in X_F° defined by $D(z,\lambda)|_F$ is singular at x_F.*

A periodic graph is dense if it has all possible edges given its structure. More specifically, if there is one edge between translates $\beta + W$ and $\gamma + W$ of the fundamental domain $W \subset \mathcal{V}(\Gamma)$ then all edges between vertices in the union $(\beta + W) \cup (\gamma + W)$ are in Γ: For each $u, v \in W$, there is an edge between $\beta + u$ and $\gamma + v$, unless $\beta = \gamma$ and $u = v$ (as our graphs do not have loops). Of the two graphs in Figure 4, the one on the left is dense. The

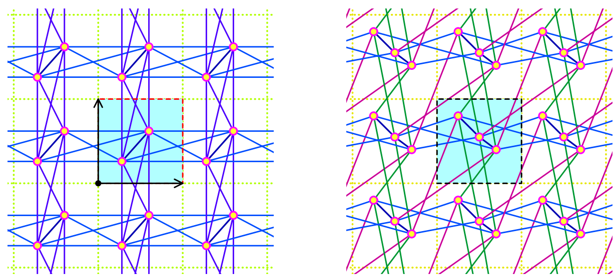

FIGURE 4. More periodic graphs.

graph on the right and the honeycomb graph (Figure 1) are not dense.

Given a graph Γ, let $A(\Gamma)$ be the set of $\gamma \in \mathbb{Z}^d$ such that Γ has an edge between W and $\gamma + W$. Let P be the convex hull of $A(\Gamma)$ and the point $(\mathbf{0}, 1)$, which is a pyramid over the convex hull Q of $A(\Gamma)$ with apex $(\mathbf{0}, 1)$. It has no vertical faces.

Theorem 4. *Suppose that Γ is dense. Then there is a dense open subset U of the space of parameters consisting of parameters c, V such that the Newton polytope P_Γ of the dispersion function $D(z,\lambda)$ is $|W| \cdot P$.*

When $d = 2, 3$, we may choose U such that for parameters c, V from U and all faces F of P_Γ, the hypersurface in X_F° defined by $D(z,\lambda)|_F$ is smooth.

While assuming that Γ is dense is sufficient for smoothness at infinity to hold, it is not necessary. The non dense graph on the right in Figure 4 (whose Newton polytope is the rightmost in Figure 3) satisfies the conclusion of Theorem 4—its generic Bloch varieties are smooth at infinity, and thus have $6 \cdot \mathrm{vol}\,\mathcal{N}(\Gamma) = 140$ critical points.

Using the formula for the volume of a pyramid, we obtain the following result.

Corollary 5. *Suppose that Γ is dense and $d = 2, 3$. Then there is a dense open subset U of the space of parameters consisting of parameters c, V such that the function λ on the complex variety has exactly $|W|^{d+1} d!\mathrm{vol}(Q)$ critical points, counted with multiplicity.*

These results are used in [9] to prove the critical points conjecture, and hence the spectral edges conjecture for many $2 + 2^{19}$ periodic graphs when $d = 2$.

4. FUTURE WORK

There are several natural lines of research that are being pursued. The operator $L(z) - \lambda I$ is a map of trivial rank $|W|$ bundles over X°. What is its extension to the toric variety X_Γ, and does this have a spectral theory interpretation? (There are hints of this in the works of Bättig, Gieseker, Knörrer, and Trubowicz [3, 12].)

The operator $L(z)$ is also a map of free modules over the ring of Laurent polynomials. How do its homological invariants relate to properties of its spectrum? Kravaris has results in this direction [16].

In [12], the compactified Bloch and Fermi varieties in X_Γ are singular, as is X_Γ. Their results are obtained after a further desingularization of X_Γ. Such desingularizations should be understood for general graphs Γ.

In [7], the spectral edges conjecture was proven for the graph on the left in Figure 4. The key step involved understanding the critical points, from which the conjecture followed by a single computation. It is reasonable to extend these arguments and results to other $\mathbb{Z}^2$-periodic graphs Γ.

In [11], the Bloch and Fermi varieties were shown to be irreducible for graphs in all dimensions similar to those studied in [12], and this has been generalized by Faust and Lopez-García [10]. Liu [20] studied the identifiability of the Fermi variety in some cases, and this is being extended in work with Faust and Liu.

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