Spectral and scattering theory for perturbed periodic graphs

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Motivation: Discrete Laplacian in $\mathbb{Z}^d$ (1)

Let us consider the discrete Laplacian on $\mathbb{Z}^d$ defined for $f \in l^2(\mathbb{Z}^d)$ by

$$(\Delta f)(\mu) = \sum_{|\gamma-\mu|=1} \left(f(\gamma) - f(\mu)\right) .$$

The discrete Fourier transform $\mathscr{F} : l^2(\mathbb{Z}^d) \to L^2(\mathbb{T}^d)$ is defined for a compactly supported f by

$$\left[\mathscr{F} f\right](\xi) = \sum_{\mu \in \mathbb{Z}^d} \mathrm{e}^{-2\pi i \xi \cdot \mu} f(\mu) .$$

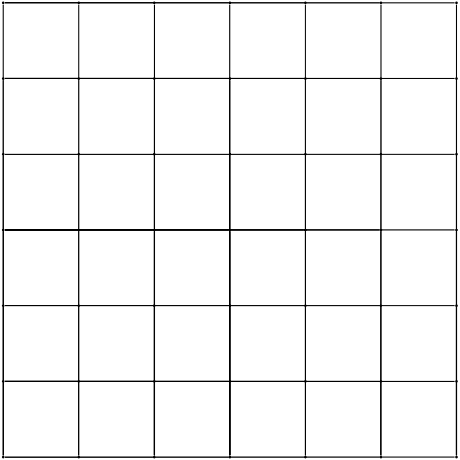
The discrete Laplacian satisfies

$$\left[\mathscr{F} \Delta \mathscr{F}^* u\right](\xi) = \left(2 \sum_{j=1}^{d} (\cos(2\pi\xi_j) - 1)\right) u(\xi) .$$

Hence, we have:

$$\sigma(-\Delta) = \sigma_{ac}(-\Delta) = [0, 2d]$$

Motivation: Discrete Laplacian in $\mathbb{Z}^d$ (2)



$$(\Delta f)(\mu) = \sum_{\gamma \sim \mu} \big(f(\gamma) - f(\mu)\big)$$

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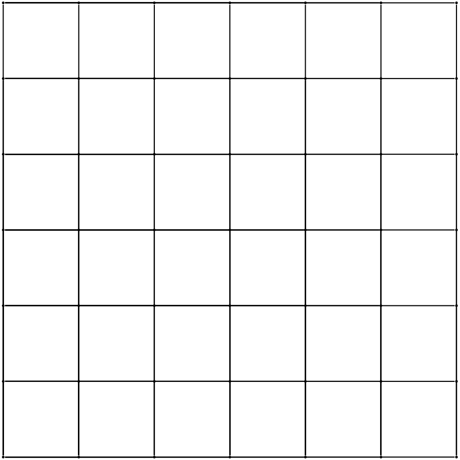

$$(\Delta' f)(\mu) = \sum_{\gamma \sim \mu} |\gamma - \mu|^{-1} \big(f(\gamma) - f(\mu) \big)$$

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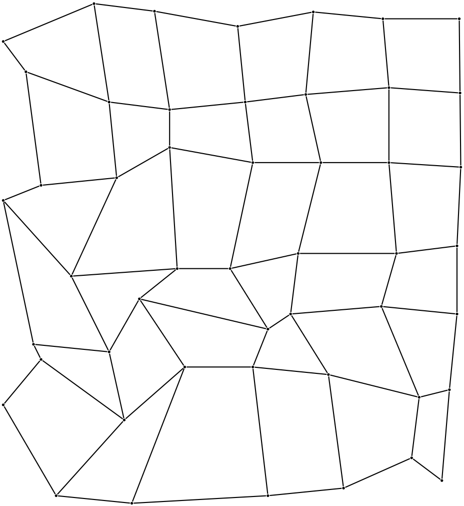

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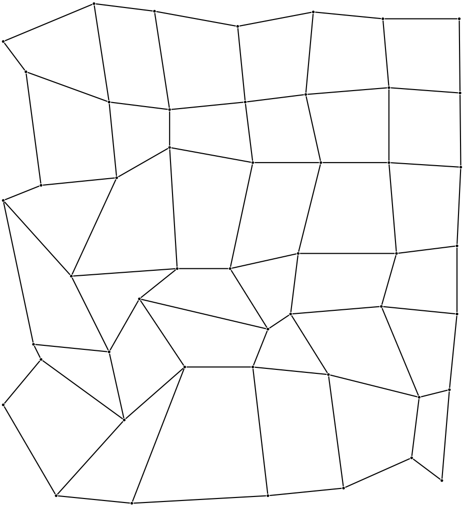

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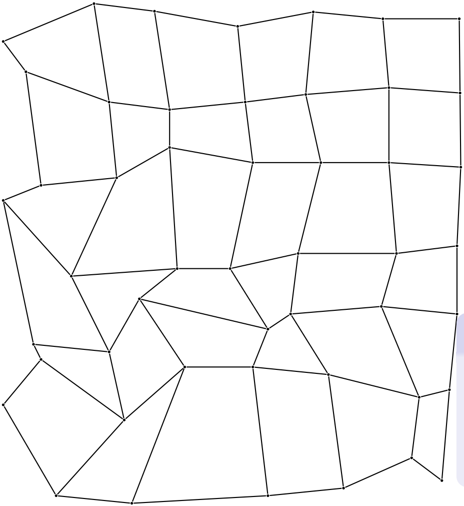

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Questions

- For which graphs this analysis is available?
- For which operators?

Outline

1. Discrete differential operators on graphs
2. Topological crystals
3. Statement of main theorem
4. Outline of the proof

The space of cochains $C(X)$

Let $X = (V(X), E(X))$ be an unoriented graph. We construct the set of oriented edges $A(X)$ by considering each $e \in E$ with two orientations *i.e.* :

$$e = \{x, y\} \in E \implies \{(x, y), (y, x)\} \subset A(X) \ .$$

We denote by $\overline{e}$ the opposite edge of e.

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We denote by $\overline{e}$ the opposite edge of e. We set

$$\begin{aligned} C^0(X) &:= \{f : V(X) \to \mathbb{C}\} \ , \\ C^1(X) &:= \{f : A(X) \to \mathbb{C} \mid f(e) = -f(\overline{e})\} \ , \\ C(X) &:= C^0(X) \oplus C^1(X) \ . \end{aligned}$$

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A measure m on X is given by two functions $m : V(X) \to (0, \infty)$ and $m : E(X) \to (0, \infty)$. We define the Hilbert space $l^2(X, m)$ as the closure of $C_c(X) = \{f \in C(X) \mid f \text{ has compact support}\}$ in the norm induced by the inner product given by

$$\langle f, g \rangle = \sum_{x \in V(X)} m(x) f(x) \overline{g(x)} + \frac{1}{2} \sum_{e \in A(X)} m(e) f(e) \overline{g(e)} \ .$$

Boundary and coboundary operators

We can now define the *coboundary operator* $d : C_c^0(X) \to C^1(X)$ by:

$$df(e) := f(t(e)) - f(o(e)).$$

We denote by $A_x = \{e \in A(X) \mid o(e) = x\}$. Then, its formal adjoint $d^* : C_c^1(X, m) \to C_c^0(X, m)$ is given by

$$d^* f(x) = -\sum_{e \in A_x} \frac{m(e)}{m(x)} f(e)$$

and corresponds to the *boundary operator*.

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and corresponds to the *boundary operator*. We can extend both operators by zero to get $d, d^* : C_c(X) \to C(X)$.

The Gauss-Bonnet operator on a graph

Then we can define the Gauss–Bonnet operator $D(X,m)$ by

$$D \equiv D(X,m) : C_c(X) \to C(X) \quad ; \quad D(X,m) := d + d^* \ .$$

It is also written in matrix form for $(f_0, f_1) \in C_c(X)$

$$\begin{pmatrix} 0 & d^* \\ d & 0 \end{pmatrix} \begin{pmatrix} f_0 \\ f_1 \end{pmatrix} = (d^* f_1, df_0)$$

Remark

We defined D in the dense subspace $C_c(X)$. It extends to a bounded operator in $l^2(X,m)$ if and only if

$$\deg_m : V(X) \to (0,\infty] \ ; \ \deg_m(x) = \sum_{e \in A_x} \frac{m(e)}{m(x)}$$

is bounded.

Laplacians on graphs

Since by definition $d^2 = 0 = (d^*)^2$ on $C(X)$, $D(X,m)$ satisfies

$$D(X,m)^2 = d^*d + dd^* = -\Delta_0(X,m) - \Delta_1(X,m)$$

where $\Delta_0(X,m)$ is the graph-Laplacian on vertices and is given by

$$\left[\Delta_0(X,m)f\right](x) = \sum_{e\in A_x} \frac{m(e)}{m(x)}\left(f(t(e)) - f(x)\right) \,,$$

and $\Delta_1(X,m)$ is the graph-Laplacian acting on edges and is given by

$$\left[\Delta_1(X,m)f\right](e) = \sum_{e'\in A_{t(e)}} \frac{m(e')}{m(t(e))} f(e') - \sum_{e'\in A_{o(e)}} \frac{m(e')}{m(o(e))} f(e') \,.$$

It follows that D should be considered like an analog of Dirac-type operators on manifolds because its square is a Laplacian-type operator.

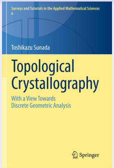
Topological crystals

Definition

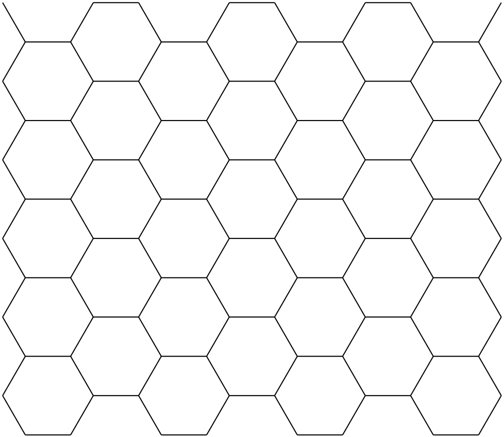
Let $X = (V(X), E(X))$ be an infinite connected graph which admits a free action of $\mathbb{Z}^d$ by graph automorphism such that $\mathfrak{X} := X/\mathbb{Z}^d$ is a finite connected graph. We say that X is a d-dimensional topological crystals over the base graph $\mathfrak{X}$.

Reference:

T. Sunada, *Topological Crystallography: With a View Towards Discrete Geometric Analysis*, Surveys and Tutorials in the Applied Mathematical Sciences, Springer, 2012.



The hexagonal lattice



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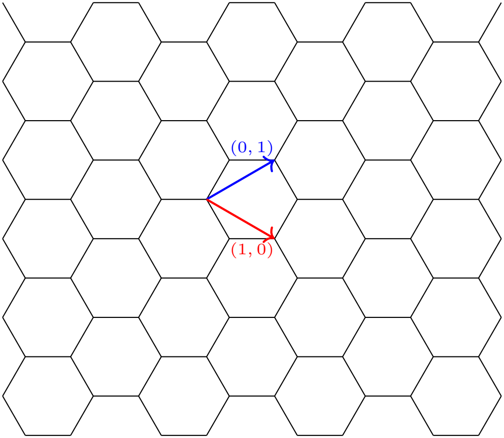

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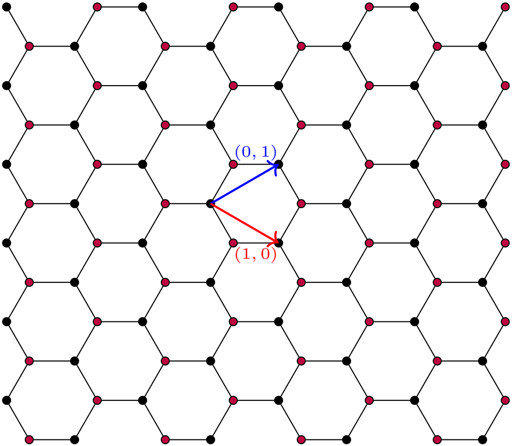

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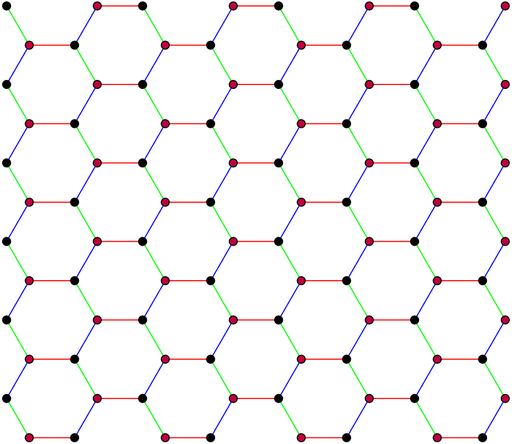

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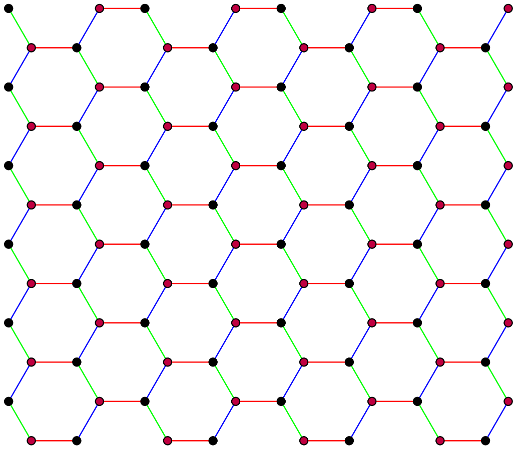

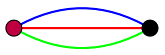

Notations for topological crystals

We start by fixing $\tilde{V} \subset V(X)$ such that $\tilde{V} \cong V(\mathfrak{X})$. Then we define $\tilde{A} \subset A(X)$ by

$$\tilde{A} = \cup_{x \in \tilde{V}} A_x \ .$$

For $\mathfrak{x} \in V(\mathfrak{X})$ we denote by $\hat{\mathfrak{x}}$ the corresponding element of $\tilde{V}$. Analogously we denote $\hat{\mathfrak{e}} \in \tilde{A}$.

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We can now define the integer part of a vertex $[x] \in \mathbb{Z}^d$ or an oriented edge $[e] \in \mathbb{Z}^d$ by the equalities

$$[x]\,\check{x} = x \quad ; \quad [e]\,\check{e} = e \quad ; \qquad \text{with } \check{x} \in \tilde{V}, \check{e} \in \tilde{A} \ .$$

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Finally we can define the index of an oriented edge by

$$\eta : A(X) \to \mathbb{Z}^d \quad ; \quad \eta(e) = [t(e)] - [o(e)]$$

One can check that η is $\mathbb{Z}^d$-periodic so we can define η also on $A(\mathfrak{X})$.

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$$\eta(e) = -\eta(\overline{e})$$

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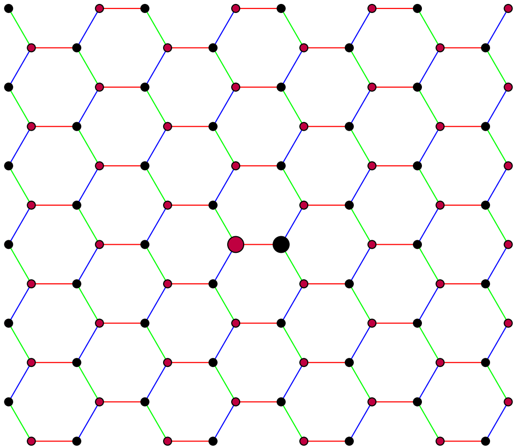

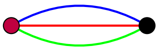

$\tilde{V} \subset V(X)$

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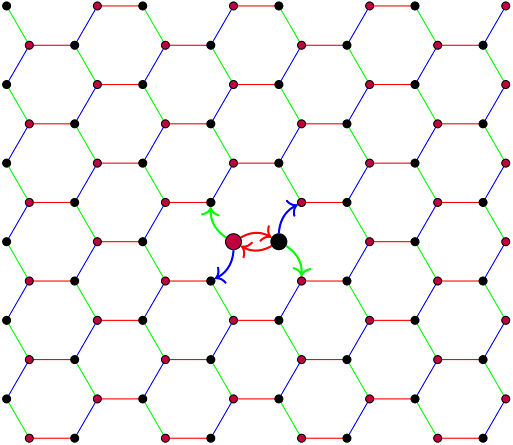

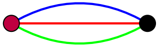

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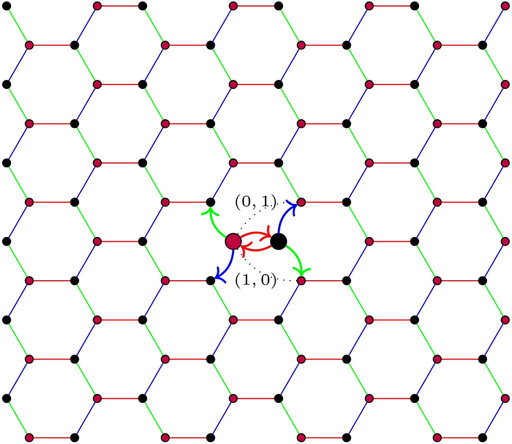
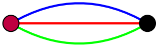


$\eta(\leftarrow) = (0,1) = -\eta(\rightarrow)$



$\eta(-) = (0,0)$

$\eta(\leftarrow) = (1,0) = -\eta(\rightarrow)$

$\eta(e) = [t(e)] - [o(e)]$

Unperturbed operators

Let X be a d-dimensional topological crystal. We fix a measure m_Γ over X such that

$$m_\Gamma(\mu x) = m_\Gamma(x) \text{ and } m_\Gamma(\mu e) = m_\Gamma(e) \ .$$

We consider also a periodic potential $R_\Gamma : X \to \mathbb{R}$ defined both in vertices and unoriented edges and define the multiplication operator associated to it by

$$[R_\Gamma f]\,(x) = R_\Gamma(x) f(x) \qquad [R_\Gamma f]\,(e) = R_\Gamma(e) f(e) \ .$$

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$$\left[R_\Gamma f\right](x) = R_\Gamma(x) f(x) \qquad \left[R_\Gamma f\right](e) = R_\Gamma(e) f(e) \ .$$

Then we will consider as unperturbed operators H_0 any of the followings bounded self-adjoint operators

$$D(X, m_\Gamma) + R_\Gamma : l^2(X, m_\Gamma) \to l^2(X, m_\Gamma) \tag{1}$$

$$-\Delta_0(X, m_\Gamma) + R_\Gamma : l_0^2(X, m_\Gamma) \to l_0^2(X, m_\Gamma) \tag{2}$$

$$-\Delta_1(X, m_\Gamma) + R_\Gamma : l_1^2(X, m_\Gamma) \to l_1^2(X, m_\Gamma) \tag{3}$$

Perturbed operators

Let now consider a measure $m \xrightarrow{x,e\to\infty} m_\Gamma$ on X. We define the unitary transform $\mathscr{I} : l^2(X,m) \to l^2(X,m_\Gamma)$ by:

$$\mathscr{I} f(x) = \left(\frac{m(x)}{m_\Gamma(x)}\right)^{\frac{1}{2}} f(x) \quad ; \quad \mathscr{I} f(e) = \left(\frac{m(e)}{m_\Gamma(e)}\right)^{\frac{1}{2}} f(e).$$

Then we will consider as perturbed operators H any of the followings bounded self-adjoint operators

$$\mathscr{I} D(X,m)\mathscr{I}^* + R_\Gamma : l^2(X,m_\Gamma) \to l^2(X,m_\Gamma) \tag{4}$$

$$-\mathscr{I}\Delta_0(X,m)\mathscr{I}^* + R_\Gamma : l^2_0(X,m_\Gamma) \to l^2_0(X,m_\Gamma) \tag{5}$$

$$-\mathscr{I}\Delta_1(X,m)\mathscr{I}^* + R_\Gamma : l^2_1(X,m_\Gamma) \to l^2_1(X,m_\Gamma) \tag{6}$$

Main statement

Theorem

Let X be a topological crystal. Let H_0 and H be defined by any of eqs. (1) *to* (3) *and eqs.* (4) *to* (6) *respectively. Assume that m satisfies*

$$\int_1^\infty \mathrm{d}\lambda \sup_{\lambda<|[e]|<2\lambda} \left| \frac{m(e)}{m(o(e))} - \frac{m_\Gamma(e)}{m_\Gamma(o(e))} \right| < \infty. \tag{7}$$

Then there exists a discrete set $\tau \subset \mathbb{R}$ such that for every closed interval $I \subset \mathbb{R}\backslash\tau$ the following assertions hold in I:

1. *H_0 has purely absolutely continuous spectrum,*
2. *H has no singular continuous spectrum and has at most a finite number of eigenvalues, each of finite multiplicity,*
3. *the local wave operators* $W_\pm \equiv W_\pm(H, H_0; I) = s - \lim_{t\to\pm\infty} e^{iHt}e^{-iH_0t}E_{H_0}(I)$ *exist and are asymptotically complete.*

Some remarks

- Condition eq. (7) is fulfilled in particular if for some constants $C, \epsilon > 0$

$$\left|\frac{m(e)}{m(o(e))} - \frac{m_\Gamma(e)}{m_\Gamma(o(e))}\right| < C|\,[e]\,|^{-1-\epsilon}$$

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- eq. (7) is the same for the three operators considered and is of *short range type*

Outline of the proof

- Using the periodicity, one can construct a unitary transform $\mathscr{U} : l^2(X, m_\Gamma) \to L^2(\mathbb{T}^d; \mathbb{C}^{n+l})$.

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- Finally one can check that eq. (7) permits to show that the difference $\mathscr{U}(H - H_0)\mathscr{U}^*$ is bounded in some convenient space from where we can deduce the properties for the Wave operators.

Conjugate Operator (1): Mourre Theory

The general idea of Mourre theory is, given a self-adjoint operator H_0 and an interval $I \subset \sigma(H_0)$, to construct a conjugate operator A_I such that for some $a > 0$ one has

$$E_I(H_0)\,[H_0, iA_I]\,E_I(H_0) \geq aE_I(H_0)$$

Such an inequality is called a *strict Mourre estimate*.
Note that for such an estimate to be meaningful we need some information on the commutator $[H_0, iA_I]$. In fact we need this commutator to be bounded, which is usually refereed to as $H_0 \in C^1(A)$. If we ask little more regularity, namely $H_0 \in C^{1,1}(A)$, a limiting absorption principle holds from which we can deduce that H_0 has absolutely continuous spectrum in I.

Conjugate Operator (2): Construction in a simple case

In our context we have $H_0 = \int_{\mathbb{T}^d}^{\oplus} H_0(\xi)$ and each $H(\xi)$ has $n+l$ eigenvalues.
As seen in the example of the Hexagonal Lattice one can hope to find analytic families of eigenvalues λ_i and associated eigenprojections Π_i outside a discrete subset of $\mathbb{T}^d$. Then a natural conjugate operator is given formally by $A := -i \sum \Pi_i \big((\nabla\lambda_i) \cdot \nabla + \nabla \cdot (\nabla\lambda_i)\big)\Pi_i$. One can see that formally the commutator is given by

$$E_I(H_0)\,[H_0, iA]\,E_I(H_0) = \sum_{\lambda_i \in I} \Pi_i |\nabla\lambda_i|^2 \Pi_i$$

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Remark

However this is not true for a general periodic graph of dimension $d > 2$. Then one need a carefully study of the Bloch variety to be able to construct a conjugate operator.

The perturbation (1)

Proposition

Let H_0 be a bounded self-adjoint operator conjugate to A_I on I and of class $C^{1,1}(A_I)$. Let V be a compact self-adjoint operator that belongs to $C^{1,1}(A_I)$. Then the operator $H_0 + V$ has at most a finite number of eigenvalues in I, and no singular continuous spectrum in I.

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We need the notion of a *toroidal pseudodifferential operator* $\mathfrak{Op}(a)$ acting on $u \in C^\infty(\mathbb{T}^d; \mathbb{C}^n)$ and given by

$$[\mathfrak{Op}(a)u](\xi) := \sum_{\mu \in \mathbb{Z}^d} e^{-2\pi i \xi \cdot \mu} a(\xi, \mu) \, \check{u}(\mu), \qquad \xi \in \mathbb{T}^d,$$

where $a : \mathbb{T}^d \times \mathbb{Z}^d \to M_n(\mathbb{C})$ is called its symbol.

The perturbation (2): Special class of regular symbols

For a bounded $a : \mathbb{Z}^d \to M_n(\mathbb{C})$ and a fixed $\nu \in \mathbb{Z}^d$, we consider the symbol $a_\nu : \mathbb{T}^d \times \mathbb{Z}^d \to M_n(\mathbb{C})$ defined by

$$a_\nu(\xi, \mu) = e^{2\pi i \xi \cdot \nu} a(\mu), \qquad \forall \xi \in \mathbb{T}^d,\ \mu \in \mathbb{Z}^d,$$

and the symbol $a_\nu^\dagger : \mathbb{T}^d \times \mathbb{Z}^d \to M_n(\mathbb{C})$ defined by

$$a_\nu^\dagger(\xi, \mu) = e^{-2\pi i \xi \cdot \nu} a(\mu + \nu)^*, \qquad \forall \xi \in \mathbb{T}^d,\ \mu \in \mathbb{Z}^d.$$

It follows that $\mathfrak{Op}(a_\nu)^* = \mathfrak{Op}(a_\nu^\dagger)$.

Lemma

Let $a : \mathbb{Z}^d \to M_n(\mathbb{C})$ be such that

$$\int_1^\infty \mathrm{d}\lambda \sup_{\lambda < |\mu| < 2\lambda} \|a(\mu)\| < \infty \ .$$

Then for any fixed $\nu \in \mathbb{Z}^d$ the operator $\mathfrak{Op}(a_\nu + a_\nu^\dagger)$ belongs to $C^{1,1}(A_I)$.

The perturbation (3)

Lemma

$\mathscr{U}(H - H_0)\mathscr{U}^*$ is a toroidal pseudodifferential operator with a symbol b that can be written as

$$b = \sum_{\mathfrak{f}} \left(b(\mathfrak{f})_{\nu_{\mathfrak{f}}} + b(\mathfrak{f})^{\dagger}_{\nu_{\mathfrak{f}}} \right) .$$

Remarks

- The set of $\{\mathfrak{f}\}$ is different for different H but it is related to $A(\mathfrak{X})$
- Each $b(\mathfrak{f})$ is a matrix with only one entry
- Then, the hypothesis of the previous Lemma can be directly deduce from our assumptions of our main result

Unitary transform (1): Magnetic operators

For any $\theta : A(\mathfrak{X}) \to \mathbb{T}$ satisfying $\theta(\bar{\mathfrak{e}}) = \overline{\theta(\mathfrak{e})}$ one sets the space of *magnetics 1-cochains* by

$$C^1(X_\theta) := \{f : A(\mathfrak{X}) \to \mathbb{C} \mid f(\bar{\mathfrak{e}}) = -\overline{\theta(\mathfrak{e})} f(\mathfrak{e})\} \ .$$

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Then the *Magnetic Gauss-Bonnet operator* $D(\mathfrak{X}_\theta, m)$ is defined by the formulae:

$$d_\theta f(\mathfrak{e}) = \theta(\mathfrak{e}) f(t(\mathfrak{e})) - f(o(\mathfrak{e})) \ ,$$

$$d_\theta^* f(x) = -\sum_{\mathfrak{e} \in A_x} \frac{m(\mathfrak{e})}{m(x)} f(\mathfrak{e}) \ .$$

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We denote by $l^2(\mathfrak{X}_\theta, m)$ the Hilbert space defined as the closure of $C_c(\mathfrak{X}_\theta, m) = C_c^0(\mathfrak{X}, m) \oplus C_c^1(\mathfrak{X}_\theta, m)$.

Unitary transform (2): Definition

Let X be a d-dimensional topological crystal. Let suppose that a measure m_Γ on X is $\mathbb{Z}^d$-periodic. Then m_Γ is also a measure on $\mathfrak{X}$.

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Lemma

Let $\mathscr{U} : C_c(X) \to \mathcal{H}$ be defined for all $\xi \in \mathbb{T}^d$, $\mathfrak{x} \in V(\mathfrak{X})$ and $\mathfrak{e} \in A(\mathfrak{X})$ by:

$$(\mathscr{U} f)(\xi, \mathfrak{x}) = \sum_{\mu \in \mathbb{Z}^d} \mathrm{e}^{-2\pi i(\xi\cdot\mu)} f(\mu\hat{\mathfrak{x}}) \quad ; \quad (\mathscr{U} f)(\xi, \mathfrak{e}) = \sum_{\mu \in \mathbb{Z}^d} \mathrm{e}^{-2\pi i(\xi\cdot\mu)} f(\mu\hat{\mathfrak{e}}) .$$

Then $\mathscr{U}$ extends to a unitary operator from $l^2(X, m_\Gamma)$ to $\mathcal{H}$.

Unitary transform (3): Differential operators trough $\mathscr{U}$

Lemma

Let (X, m) be a weighted topological crystal. Then

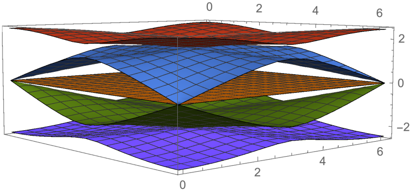
$$\mathscr{U}\, D(X, m_\Gamma)\mathscr{U}^* = \int_{\mathbb{T}^d}^{\oplus} \mathrm{d}\xi\, D(\mathfrak{X}_{\theta_\xi}, m_\Gamma) \ ,$$
$$\mathscr{U}\, \Delta_0(X, m_\Gamma)\mathscr{U}^* = \int_{\mathbb{T}^d}^{\oplus} \mathrm{d}\xi\, \Delta_0(\mathfrak{X}_{\theta_\xi}, m_\Gamma) \ ,$$
$$\mathscr{U}\, \Delta_1(X, m_\Gamma)\mathscr{U}^* = \int_{\mathbb{T}^d}^{\oplus} \mathrm{d}\xi\, \Delta_1(\mathfrak{X}_{\theta_\xi}, m_\Gamma) \ .$$

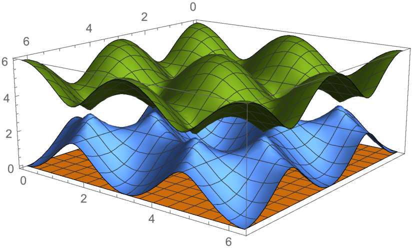
Remark

Since $\dim l^2(\mathfrak{X}_{\theta_\xi}, m) = \sharp V(\mathfrak{X}) + \sharp E(\mathfrak{X})$, and setting $n := \sharp V(\mathfrak{X})$ and $l := \sharp E(\mathfrak{X})$ we get

$$\mathcal{H} \cong L^2(\mathbb{T}^d; \mathbb{C}^{n+l})$$

Unitary transform (4): Once again, back to the hexagonal lattice





$\sigma(D(\xi)) \quad \xi \in \mathbb{T}^2$

$\sigma(\Delta_1(\xi)) \quad \xi \in \mathbb{T}^2$

Conjugate Operator (3): General determination of τ

The Bloch variety is defined by $\Sigma = \{(\lambda, \xi) \in \mathbb{R} \times \mathbb{T}^d : \lambda \in \sigma(H_0(\xi))\}$. We start by defining

$$\Sigma_j := \{(\lambda, \xi) \in \mathbb{R} \times \mathbb{T}^d \mid \lambda \text{ is an eigenvalue of } h(\xi) \text{ of multiplicity } j\} \ .$$

Since $p_{\mathbb{R}} : \mathbb{R} \times \mathbb{T}^d \to \mathbb{R}$ is real analytic there exist a stratification $(\mathcal{S}, \mathcal{S}')$ of $p_{\mathbb{R}}$ compatible with the subanalytic family $\{\Sigma_j\}$.

$$\tau := \bigcup_{\dim \mathcal{S}'_\beta = 0} \mathcal{S}'_\beta \ .$$

τ is discrete and since we are in the bounded case is indeed finite.

Conjugate Operator (4): Construction of A_I

We fix a closed interval $I \subset \mathbb{R}\backslash\tau$. For a fixed $(\lambda_0, \xi_0) \in \Sigma$, with $\lambda_0 \in I$, we define on $C_c^\infty(\mathcal{T}_0; \mathbb{C}^{n+l})$:

$$A_{\lambda_0,\xi_0} = \frac{-i}{2}\pi_{I_0}\left[(\nabla^{(s)}\boldsymbol{\lambda})\cdot\nabla^{(s)} + \nabla^{(s)}\cdot(\nabla^{(s)}\boldsymbol{\lambda})\right]\pi_{I_0} \ ,$$

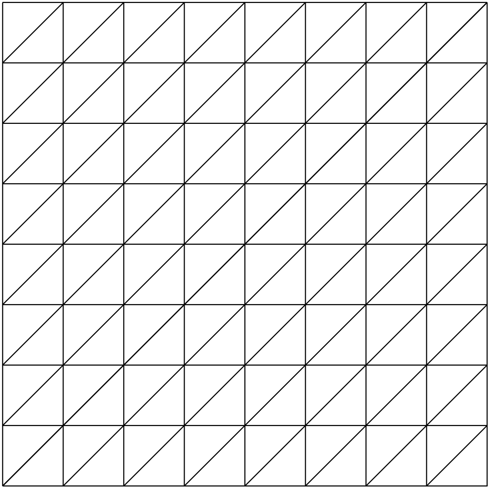
where:

- $\mathcal{T}_0$ is a conveniently chosen neighborhood of ξ_0
- I_0 is a conveniently chosen neighborhood of λ_0
- s is the dimension of $\mathcal{S}_\alpha \ni (\lambda_0, \xi_0)$
- $\boldsymbol{\lambda} : \mathbb{T}^d \to \mathbb{R}$ describes locally $\mathcal{S}_\alpha$

$$A_{\xi_0} := \sum_{\lambda_j \in \sigma(H_0(\xi_0))\cap I} A_{\lambda_j,\xi_0} \quad ; \quad A_I := \sum_\ell \chi_\ell A_{\xi_\ell}\chi_\ell$$

Where $\cup_\ell \mathcal{T}_\ell$ cover $p_{\mathbb{T}^d}(p_{\mathbb{R}}^{-1}(I))$ and $\{\chi_\ell\}$ is an associated partition of unity.

Other examples (1): The Triangular lattice



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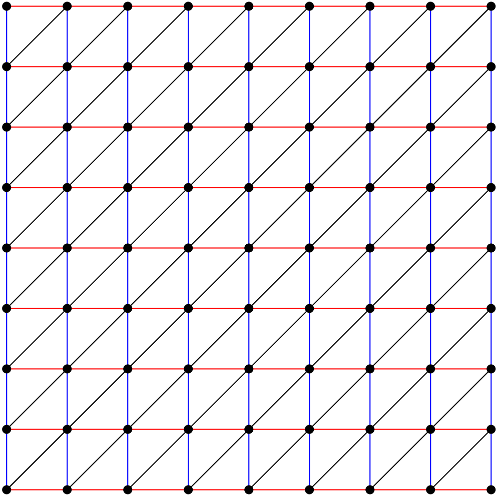

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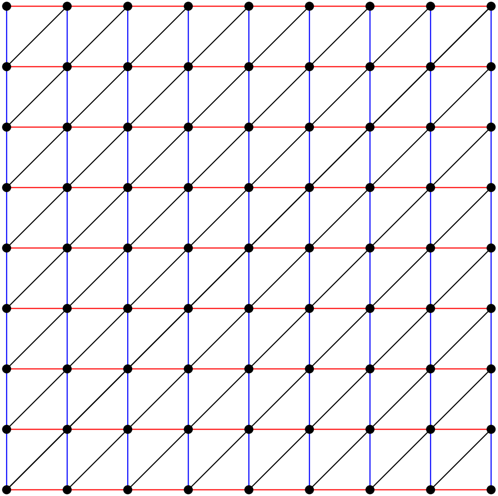

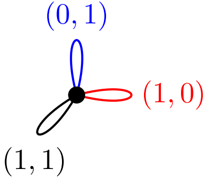

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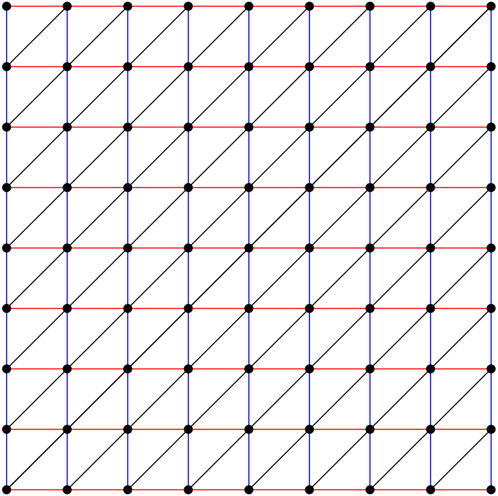
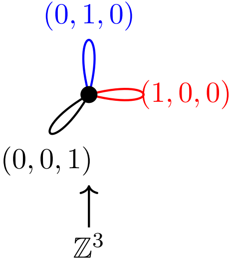
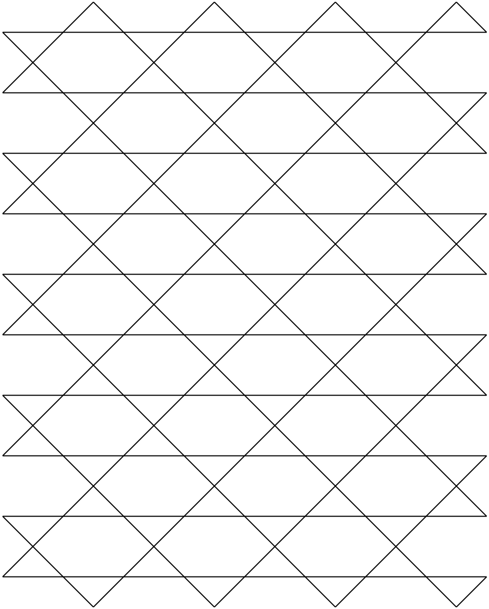




Other examples (2): The Kagome lattice



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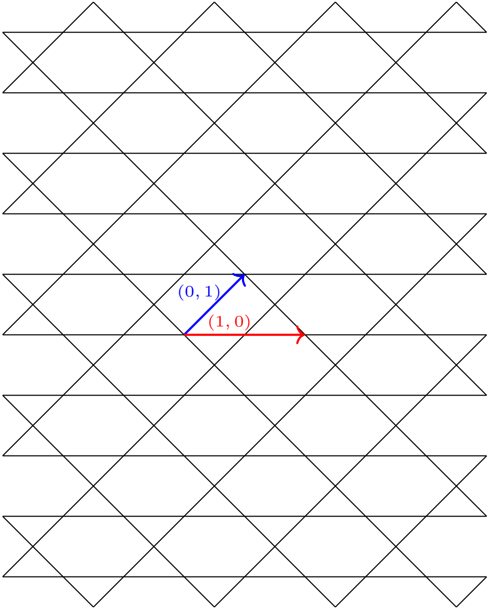

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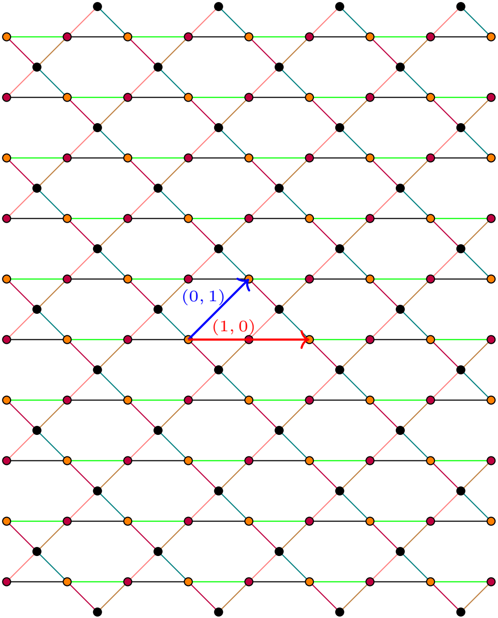

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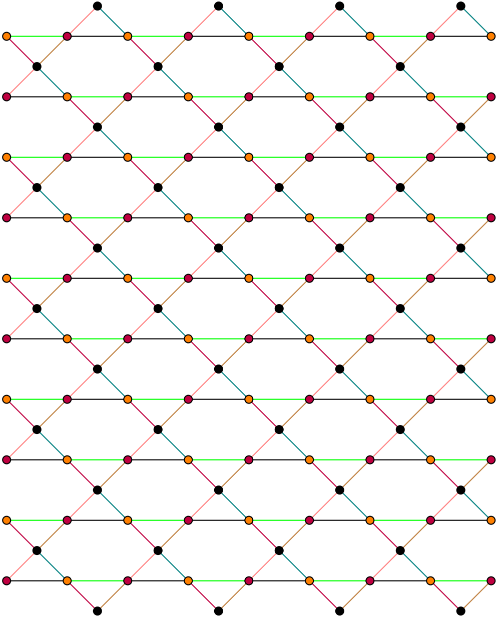

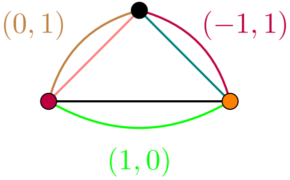

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