Singularities, swallowtails and topological properties in families of Hamiltonians

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References

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What can happen if a chemist calls . . .

Initial question by Hugh Hillhouse (Purdue, now Univ. of Wash.)

What can mathematicians and physicists tell us about our novel material, which is in the form of a Double Gyroid? What follows from its wonderful mathematical structure?

Hope

The material can be used in solar cells to make them more effective (e.g. through multiple excitations)

Outline

The Gyroid

Single Gyroid

- The Gyroid is an embedded CMC surface in $\mathbb{R}^3$.
- It was discovered by Alan Schoen in 1970.
  [NASA TN-D5541 (1970)] .
- In nature it was first observed as an interface for di-block co-polymers.
  [D. A. Hajduk et. al. 1994, M. F. Schulz, et. al 1994]
- It can be embedded.
  [K. Große–Brauckmann and M. Wohlgemuth 1994].
- A single Gyroid has high symmetry group ($I4_132$ in the international or Hermann–Mauguin notation). We will need the translation group I that is bcc.
- Level surface approximation [C. A. Lambert, L. H. Radzilowski, E. L. Thomas, 1996] (used in many pictures)
  $L_t : \sin x \cos y + \sin y \cos z + \sin z \cos x = t$

Gyroid

The Double Gyroid

The Double Gyroid (DG)

- The DG interface actually consists of *two* mutually non–intersecting embedded Gyroids.
- The symmetry group is $Ia\bar{3}d$ where the extra symmetry comes from interchanging the two Gyroids. This is used to identify the structure in crystallography.
- A level surface model for the double Gyroid is given by L_w and L_{-w} for $0 \leq w < \sqrt{2}$

Thick surface

The picture was actually a DG. That is a "thick" or "fat" gyroid surface.

Channels and fat surface

Regions

Let $S = S_1 \amalg S_2$ be the DG.
$C = \mathbb{R}^3 \setminus S$ has three connected components: C_+, C_-, F

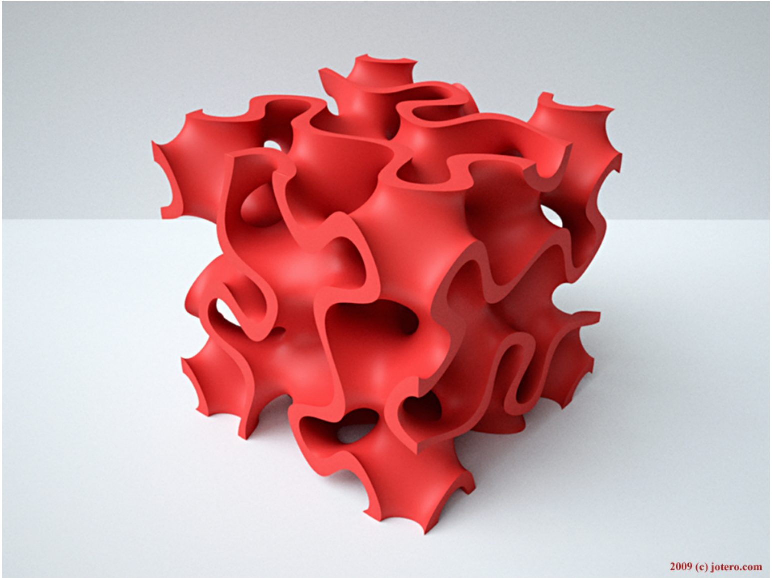
Channels

There are two channel systems C_+ and C_-, each of which can be deformation retracted to a skeletal graph $\Gamma_\pm$.

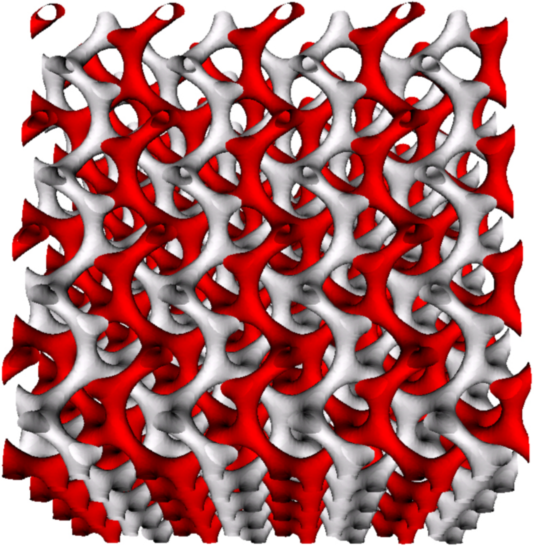
Fat surface

There is a third connected component F .
$\bar{F} = F \cup S$ is a 3-manifold with two boundary components, $\partial\bar{F} = S = S_1 \amalg S_2$.
F can be thought of as a "thickened" (fat) surface. The thickness is fixed by the parameter w. There is a deformation retract of F onto a single Gyroid.

The fat surface F



The two channel systems C_+, C_-



The two channel systems C_+, C_-: one cell

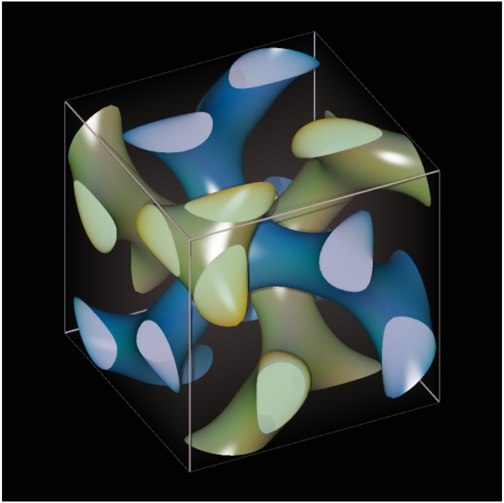


Figure: The two channel systems

The Channel C_+

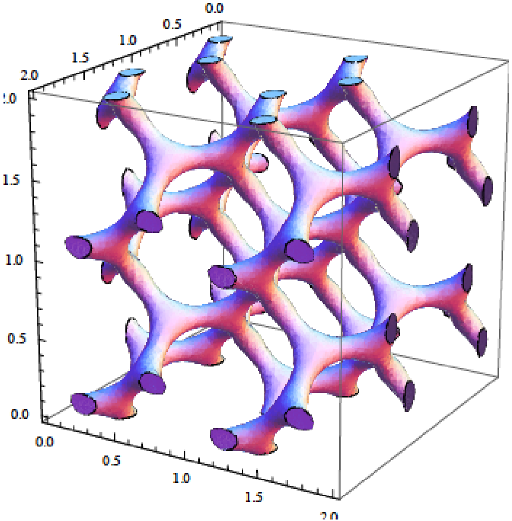
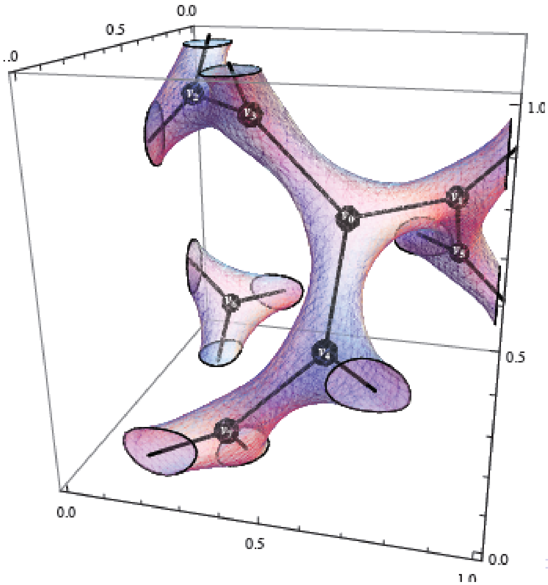
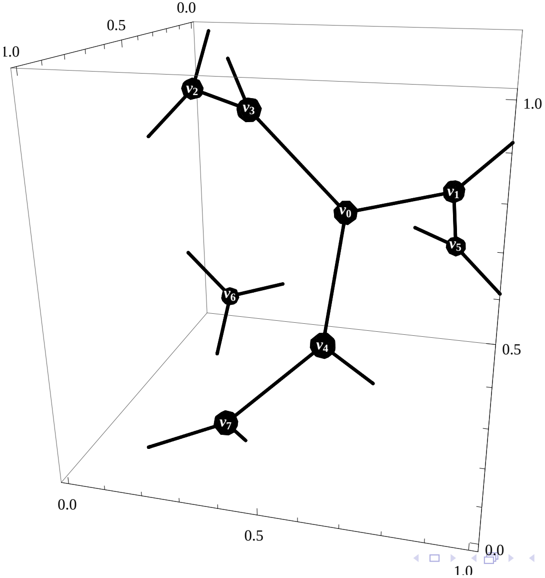


Figure: One channel

The Channel C_+ with its skeletal graph Γ_+



The skeletal graph Γ_+



Fabrication

Hugh Hillhouse et al., Purdue now Univ. of Washington.

- Semiconductor quantum-wire arrays of PbSe, PbS, and CdSe have been synthesized via self–assembly.
- The first synthesis step yields a nanoporous silica structure – the fat surface. The nanopores (channels) are then filled with a semiconductor and the fat surface is dissolved to yield the nanowire network.
- After making a DG wire structure a second semiconductor material may potentially be grown in the void space to yield a bulk heterojunction semiconductor.

Dimensions and quantum wires

- DG lattice constant: 18nm
- Quantum effects in wire with semi-conductor below 100nm
- Related material graphene has bond length 0.142nm

Measurements: Eric Stach, Purdue, now Brookhaven Nationl. Lab.

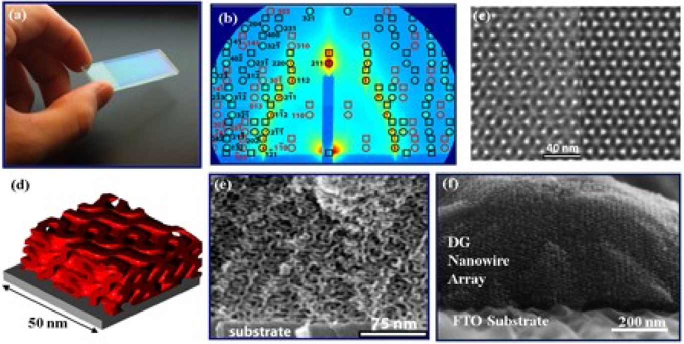


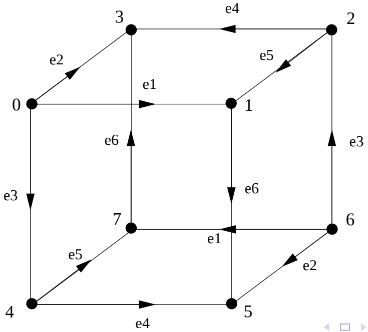
Figure: (a) Photograph of DG nanoporous silica film on FTO after self-assembly and surfactant extraction. (b) GISAXS from film showing the high-degree of order and orientation. (c) TEM image of the (111) projection of the DG nanoporous silica film compared with a simulated TEM image for the DG structure. (d) Quantitatively accurate structure of the DG nanoporous silica films determined by GISAXS and TEM. (e) High resolution FESEM image of the cross section of a film. The patterns seen in the structure in panel (d) are easily seen. (f) DG platinum nanowire array obtained by electrodepositing Pt in the DG nanoporous film followed by etching in HF or KOH. Periodic y-junctions can be seen in the nanowires extending from top to bottom through the film.

Topology of C_+ or Γ_+: finite quotients

Since Γ_+ is a deformation retract, we get the same homotopical information as for C_+.

Quotient by the translational group $\mathbb{Z}^3 \subset \mathbb{R}^3$

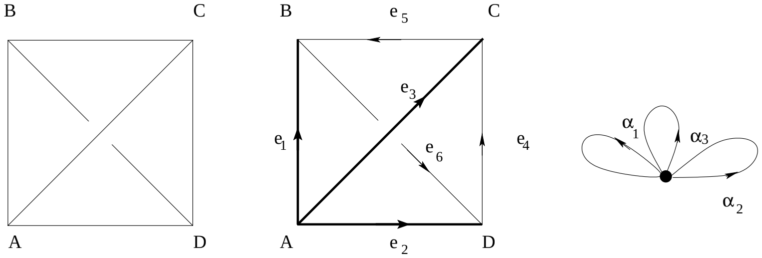
$\Gamma_+/\mathbb{Z}^3$ is a cube. The eight vertices are the images of the vertices $v_0, \ldots, v_7$.



Topology of C_+ or Γ_+: finite quotients

Quotient by the full translational symmetry group: bcc

The body centered cubic (bcc) lattice group is generated by
$f_1 := (1,0,0), \quad f_2 = (0,1,0), \quad f_3 := \frac{1}{2}(1,1,1)$. Or
$g_1 = \frac{1}{2}(1,-1,1), \quad g_2 = \frac{1}{2}(-1,1,1), \quad g_3 = \frac{1}{2}(1,1,-1)$
$\bar{\Gamma}_+ := \Gamma_+/bcc$ is a tetrahedron or full square. This is obtained from the cube by identifying opposite corners
$v_0 \leftrightarrow v_6, v_1 \leftrightarrow v_7, v_2 \leftrightarrow v_4$ and $v_3 \leftrightarrow v_5$.



C^*–geometry

Connes–Bellissard–Harper approach

Replace the geometric setup with a C^* algebra $\mathscr{B}$ which is the smallest algebra containing the Hamiltonian and the symmetries. The standard choice of the Hamiltonian is the Harper Hamiltonian. This acts on the Hilbert space $\mathscr{H} = \ell^2(\Lambda)$ where Λ are the vertices.

General setup

$\Gamma \subset \mathbb{R}^n$ a connected embedded graph.
L a (maximal) translational symmetry group of Γ, s.t.
$\bar{\Gamma} = \Gamma/L$ is finite. $\pi : \Gamma \to \bar{\Gamma}$ the projection.
Λ be the set of vertices of Γ, $\bar{\Lambda}$ the set of vertices of $\bar{\Gamma}$.
$T =$ (free Abelian) subgroup of $\mathbb{R}^n$ generated by the edge vectors.
Notice $L \subset T$.

Actions

Hilbert space

$\mathscr{H} = \ell^2(\Lambda) = \bigoplus_{\bar{v}\in\bar{\Lambda}} \mathscr{H}_{\bar{v}}$ where $\mathscr{H}_{\bar{v}} = \ell^2(\pi^{-1}(\bar{v}))$

Action of L

L acts via translation operators on $\mathscr{H}$:
For $l \in L$: $T_l(\phi)(v) = \phi(v - l)$.
This action is by isometries and it maps: $\mathscr{H}_{\bar{v}} \to \mathscr{H}_{\bar{v}}$.

Operations defined by T (it does not act on $\mathscr{H}$ in general)

T only acts by partial isometries. If $\vec{e}$ is a directed edge whose image under π is from $\bar{v}$ to $\bar{w}$, then the translation yields an operator $T_{\vec{e}} : \mathscr{H}_{\bar{w}} \to \mathscr{H}_{\bar{v}}$. This extends to an operator $\hat{T}_{\vec{e}}$ on $\mathscr{H}$ via $\hat{T}_{\vec{e}} = i_{\bar{v}} T_{\vec{e}} P_{\bar{w}}$ where $i_{\bar{v}} : \mathscr{H}_{\bar{v}} \to \mathscr{H}$ is the inclusion and $P_{\bar{w}} : \mathscr{H} \to \mathscr{H}_{\bar{w}}$ is the projection.

Harper Operator

Definition

Let E be the edges of $\bar{\Gamma}$. Each directed edge defines a unique vector $\vec{e} \in \mathbb{R}^n$. Each edge e defines two directed edges and vectors $\vec{e}, -\vec{e}$.The Harper Hamiltonian is:

$$H = \sum_{e \in E} \hat{T}_{\vec{e}} + \hat{T}_{-\vec{e}}$$

If we turn on a constant background magnetic field B (a constant two form $\leftrightarrow$ skew matrix Θ), we use magnetic translations U. These do not commute in general, so everything becomes a non-commutative geometry.

$$\boxed{H = \sum_{e \in E} U_{\vec{e}} + \hat{U}_{-\vec{e}}}$$

Physics

Physics background

Use Weyl quantization and Peierls substitution. In the magnetic case (below) the magnetic translations were introduced by Wannier. And the magnetic field gives rise to a projective representation whose commutators include the fluxes of the magnetic field.

Generalization

Quiver representation

Given a finite graph $\bar{\Gamma}$, let ρ' be a functor from the path groupoid $\pi_1\bar{\Gamma}$ to separable Hilbert spaces. That is $\mathscr{H}_v$ for each $v \in V(\bar{\Gamma})$ and an isometry $U_{\vec{e}} : \mathscr{H}_v \to \mathscr{H}_w$ for each directed edge $\vec{e}$ from v to w.

Harper Hamiltonian

$$H = \sum_{e \in E(\bar{\Gamma})} \left(U_{\vec{e}} + U_{\overleftarrow{e}} \right) \in B(\mathscr{H})$$

Geometry

Geometry

Picking a base point, we get a rep of $\pi_1(\bar{\Gamma}, v_0)$, which generates a C^*–algebra $\mathscr{A}$. Adding in H we get the algebra $\mathscr{B}_0$. We get a non–commutative geometry $\mathscr{A} \hookrightarrow \mathscr{B}_0$.

Commutative geometry

In the commutative case we get a family of Hamiltonians from H over a base T ($\mathscr{A} \simeq C^*(T)$) and $\mathscr{B}_0$ corresponds to the cover X given by the Eigenvalues. I.e. the C^*–geometry describes the cover $X \to T$.

Results [KKWK] non-commutative

Expectation

Generically expect that $\mathcal{B}_0 = M_k(\mathbb{T}_\Theta) \sim_{Morita} \mathbb{T}_\Theta$. $k = \#vertices$.

Theorem [KKWK]

This is true for PDG surfaces and the honeycomb and we classified the locus where $\mathscr{B}_0$ is a proper subalgebra. Also at rational B–field there are only finitely many gaps in the spectrum (Hofstadter's butterfly).

Commutative case [KKWK]

X is a branched cover of T. For the lattice case $T = T^n$ and the cover is generically unramified. We gave the ramification locus and branching for PDG and the honeycomb.

Example 1: The Bravais lattice case aka. $\mathbb{Z}^n$

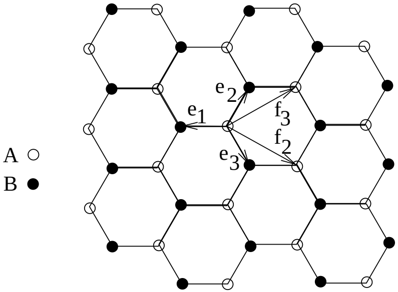
Setup

- $T = L = \mathbb{Z}^n$
- Magnetic translations: $U_i := U_{e_i}$ generate. Relations $U_i U_j = e^{2\pi i \Theta_{ij}} U_j U_i$.
- $H = \sum_i U_{e_i} + U^*_{e_i}$: $H \in$ algebra generated by the magnetic translations.

Result

The Bellissard-Harper algebra is $\mathscr{B} = \mathbb{T}^n_\Theta$. The non–commutative n–torus.

Example 2: The Honeycomb lattice aka. Graphene



Setup

The honeycomb lattice is a subset of the lattice generated by $-e_1 := (1,0)$ and $e_3 := \frac{1}{2}(1,-\sqrt{3})$. Set $e_2 = -e_1 - e_3 = \frac{1}{2}(1,\sqrt{3})$.

- $L \simeq \mathbb{Z}^2$ generated by $f_2 := e_2 - e_1 = \frac{1}{2}(-3,\sqrt{3})$ and $f_3 := e_3 - e_1 = \frac{1}{2}(3,\sqrt{3})$.
- T is generated by the e_i

The Honeycomb lattice II

The Harper Operator

$\mathscr{H} = \mathscr{H}_A \oplus \mathscr{H}_B$ and $U_{e_i} : \mathscr{H}_B \to \mathscr{H}_A$. Fix the magnetic field by $\phi = \hat{\Theta}(-e_1, e_2)$, $\chi := e^{i\pi\phi}$.

Set $\hat{U}_i := \begin{pmatrix} 0 & 0 \\ U_{e_i} & 0 \end{pmatrix}$, $\quad \hat{U}_{-i} := \begin{pmatrix} 0 & U_{-e_i} \\ 0 & 0 \end{pmatrix}$

where U_{e_i} and $U_{-e_i} = U_{e_i}^{-1} = U_{e_i}^*$ are the isomorphisms between $\mathscr{H}_A$ and $\mathscr{H}_B$.

The Harper Hamiltonian now reads:

$$H = \sum_{i=1}^{3} \hat{U}_i + \hat{U}_i^{-1} = \begin{pmatrix} 0 & U_{e_1}^* + U_{e_2}^* + U_{e_3}^* \\ U_{e_1} + U_{e_2} + U_{e_3} & 0 \end{pmatrix}$$

The Honeycomb lattice III

The Matrix Harper Operator

Fixing bases, we obtain the matrix expression:

$$H = \begin{pmatrix} 0 & 1+U^*+V^* \\ 1+U+V & 0 \end{pmatrix} \in M_2(\mathbb{T}^2_\theta)$$

where we have used the operators $U := \chi U_{f_2}$ and $V = \bar{\chi} U_{f_3}$ which satisfy $UV = qVU$ with $q := e^{2\pi i\theta} = \bar{\chi}^6$ where $\theta = \hat{\Theta}(f_2, f_3)$

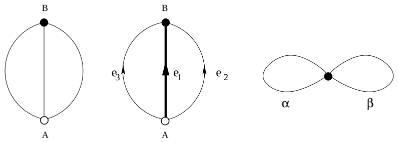


Figure: The graph $\bar{\Gamma}$, a choice of oriented edges and a spanning tree τ, $\bar{\Gamma}/\tau$

The algebra $\mathscr{B}$ in the honeycomb case

Theorem

If $q \neq \pm 1$ *or* $q = -1$ *and* $\chi^4 \neq 1$ *then* $\mathscr{B}_\Theta = M_2(\mathbb{T}^2_\theta)$ *and hence is Morita equivalent to* $\mathbb{T}^2_\theta$.
If $q = -1$ *and* $\chi^4 = 1$ *or if* $q = 1$ *and* $\chi \neq \pm 1$ *then* $\mathscr{B}_\Theta$ *is a proper subalgebra of* $M_2(\mathbb{T}^2_{\frac{1}{2}})$ *(which we know).*
If $q = 1$ *and* $\chi = \pm 1$ *then* $\mathscr{B}_\Theta = C^*(X)$ *where* X *is the double cover of the torus* $S^1 \times S^1$ *ramified at the points* $(e^{2\pi i \frac{1}{3}}, e^{2\pi i \frac{2}{3}})$ *and* $(e^{2\pi i \frac{2}{3}}, e^{2\pi i \frac{1}{3}})$.

Remark

The two ramification points play a special role in graphene where they are known as Dirac points.

Example 3: The Gyroid case

Data

- L for Γ_+ is the bcc lattice spanned by the vectors f_i or g_i.
- T is the fcc lattice spanned by the edge vectors e_4, e_5, e_6.
- In Hilbert space decomposition the Graph Harper Operator H becomes the 4×4 matrix

$$H = \begin{pmatrix} 0 & U_1^* & U_2^* & U_3^* \\ U_1 & 0 & U_6^* & U_5 \\ U_2 & U_6 & 0 & U_4 \\ U_3 & U_5^* & U_4^* & 0 \end{pmatrix}$$

- Magnetic Field Parameters:

$$\theta_{12} = \frac{1}{2\pi} B\cdot(g_1 \times g_2), \theta_{13} = \frac{1}{2\pi} B\cdot(g_1 \times g_3), \theta_{23} = \frac{1}{2\pi} B\cdot(g_2 \times g_3)$$

The Gyroid case

The matrix Harper Operator

$$H = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & U_1^* U_6^* U_2 & U_1^* U_5 U_3 \\ 1 & U_2^* U_6 U_1 & 0 & U_2^* U_4 U_3 \\ 1 & U_3^* U_5^* U_1 & U_3^* U_4^* U_2 & 0 \end{pmatrix} =: \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & A & B^* \\ 1 & A^* & 0 & C \\ 1 & B & C^* & 0 \end{pmatrix}$$

The coefficients can be expressed in terms of the operators of the magnetic translation operators of the bcc lattice. Set $U := U_{f_1}, V := U_{f_2}$ and $W := U_{f_3}$.

$$A = aV^* W, \quad B = bWU^*, \quad C = cW^* UV \tag{1}$$

with a, b, c given explicitly in terms of the magnetic field. A, B, C span a $\mathbb{T}^3_\Theta$:

$$AB = \alpha_1 BA, \quad AC = \bar{\alpha}_2 CA, \quad BC = \alpha_3 CB$$

Results for the Gyroid

Theorem

If $\Phi \neq 1$ or $\Phi = 1$ and at least one $\alpha_i \neq 1$ and all ϕ_i are different then $\mathscr{B}_\Theta = M_4(\mathbb{T}^3_\Theta)$ and $K(\mathscr{B}_\Theta) = K(\mathbb{T}^3)$.
If $\phi_i = 1$ for all i (commutative case) then $K(\mathscr{B}_\Theta) = K(X)$ where X is a ramified cover of the 3–torus with explicitly given ramification locus (consisting of four isolated points).
In all other cases $\mathscr{B}_\Theta \subsetneq M_4(\mathbb{T}^3_\Theta)$.

Parameters

$\alpha_1 := e^{2\pi i\theta_{12}}, \bar{\alpha}_2 := e^{2\pi i\theta_{13}}, \alpha_3 := e^{2\pi i\theta_{23}}$
$\phi_1 = e^{\frac{\pi}{2}i\theta_{12}}, \quad \phi_2 = e^{\frac{\pi}{2}i\theta_{31}}, \quad \phi_3 = e^{\frac{\pi}{2}i\theta_{23}}, \quad \Phi = \phi_1\phi_2\phi_3$

Commutative case

Basic questions

1. Classify the points on the base over which the Hamiltonian has degenerate Eigenvalues and give the multiplicities.
2. If possible identify symmetries, which can correspond to these Eigenspaces

Answer to Question 1

We answered Question 1 in terms of singularity theory.

Answer to Question 2

We defined a quasi–classical lift of the classical symmetries of $\bar{\Gamma}$ on the base space. This also gives rise to a representation of a group extension on $\mathbb{C}^k$ where $k = |\bar{\Lambda}|$.

Questions

Empirical data

In all cases, the degenerate points are the ones one can compute from the projective action of graph symmetries. There seems to be no *a priori* proof however. Not even for the dimension of this locus.

Duality?

In all cases, the (maximal) dimension of the locus of enhanced symmetries in the commutative case coincides with the dimension of the locus of points where $\mathscr{B}_\Theta$ is not the full matrix algebra.

New method for analytically finding degeneracies and Dirac points

Setup

- In the commutative case we get a family of Hamiltonians parameterized over a base torus T^n.
- Consider $det(z\,Id - H(t))$ as smooth function $P : T^n \times \mathbb{R} \to \mathbb{R}$.
- Determine the critical points of P, viz. singularities.
- The singularity is conical/Dirac if P has an isolated critical point and the signature of the Hessian is $(- \cdots - +)$
- Notice we use the embedding of the possibly singular spectrum $P^{-1}(0)$ into the smooth ambient space $T^n \times \mathbb{R}$.

New method for analytically finding degeneracies and Dirac points

Characteristic map

Actually $P^{-1}(0)$ is the pull–back of the miniversal unfolding of the A_{k-1} singularity along the map given by the coefficients of P considered as a polynomial in z. We call that map the characteristic map[a].

- The characteristic map lets one read off the type of singularities. They are determined by the image and the fiber.
- Singular points are inverse images of the discriminant locus.
- The type of singularity pulled back to the fiber is given by the respective stratum of the unfolding which were determined by Grothendieck.

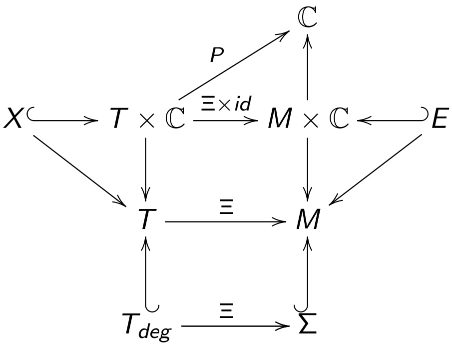
[a] There is a rescaling involved if $H(t)$ is not traceless.

Details

Characteristic map and pull-back

- $H : T \to Herm^k$ be a (smooth) family of (traceless) Hermitian $k \times k$ matrices
- $P(t) = det(z - H(t)) = z^k + a_{k-2}z^{k-2} + \cdots + a_0 z_0$.
- $\Xi : T \to \mathbb{C}^{k-2}$ be the map $t \mapsto (a_{k-2}, \ldots, a_0)$
  $\mathbb{C}^{k-2} = M_{A_{k-1}}$ is the base of the miniversal unfolding of A_{k-1}.
- $X := P^{-1}(0)$, the branched cover given by the spectrum.
- $X = \Xi^{-1}(E)$ pull–back of the universal cover of the miniversal unfolding.
- Σ swallowtail or discriminant locus. Singularities over fibers over Σ given by Grothendieck (delete vertices from Dynkin diagram $\rightsquigarrow$ stratification).
- $T_{deg} := \Xi^{-1}(\Sigma)$ singularity locus. Fibers over $\Xi^{-1}(\Sigma)$ are singular. Singularities given by codim of Ξ and Grothendieck classification.

The spaces



Results for Examples 2 and 3:

Honeycomb

In the case of $B = 0$ there are two degenerate points in the spectrum, which are cone–like/viz. Dirac. These correspond to enhanced classical symmetries.

Gyroid

In the case of $B = 0$ there are four degenerate points in the spectrum. Two of them are triple degeneracies and two of them are two double degeneracies, the latter are cone–like/viz. Dirac. These correspond to enhanced classical symmetries.

Gyroid and the A_3–Discriminant

The eigenvalues of H are given by the roots of the characteristic polynomial: $P(a,b,c,z) = z^4 - 6z^2 + a_1(a,b,c)z + a_0(a,b,c)$

$a_1 = -2\cos(a) - 2\cos(b) - 2\cos(c) - 2\cos(a+b+c)$

$a_0 = 3 - 2\cos(a+b) - 2\cos(b+c) - 2\cos(a+c)$

where $A \mapsto \exp(ia)$, $B \mapsto \exp(ib)$, $C \mapsto \exp(ic)$

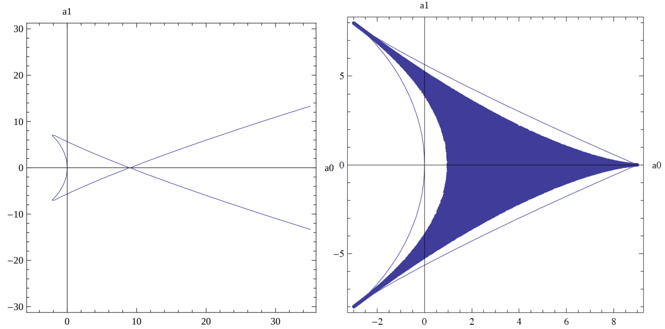


Figure: Swallowtail and region occupied by Gyroid

Gyroid: A_3 singularity and its strata

- Characteristic region contained in the slice of the A_3 singularity with $a_2 = -6$, intersects discriminant locus in three isolated points
- two cusps: in stratum of type A_2
- double point: in stratum of type (A_1, A_1)
- fibers over all points are discrete; for A_2 singularities: one point each; for (A_1, A_1): two points each; explains crossings in spectrum

Theorem [KKWK]

The singular points of X for the Gyroid are given exactly by the above (analytically). And the four A_1 singularities are all Dirac points.

The spectrum of the Gyroid Harper Hamiltonian along the diagonals

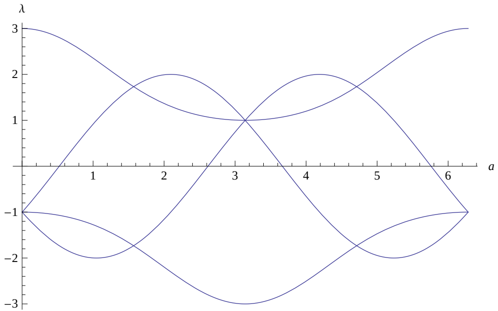


Figure: Spectrum of Harper Gyroid Hamiltonian for $a = b = c$

Basic setup

Bundle geometry

- $H : T \to Herm^k$. Universal action $Herm^k \times \mathbb{C}^k \to \mathbb{C}^k$.
- Trivial vector bundle $T \times \mathbb{C}^k \to \mathbb{C}^k$.
- T_{deg} be the locus of points s.t. $H(t)$ has multiple Eigenvalues. $T_0 := T \setminus T_{deg}$.
- $$\begin{array}{ccccc} T \times \mathbb{C}^k & \hookleftarrow & T_0 \times \mathbb{C}^k & \xrightarrow{\sim} & \bigoplus_{i=1}^k \mathscr{L}_i \\ \downarrow & & \downarrow & \swarrow & \\ T & \hookleftarrow & T_0 & & \end{array}$$

  Need that Eigenvalues are real.
- $c_1(\mathscr{L}_i)$ are the charges corresponding to the Berry phases. Integral over Berry curvature ω [Berry, Simon].

Basic setup

Bundle geometry

- $H : T \to Herm^k$. Universal action $Herm^k \times \mathbb{C}^k \to \mathbb{C}^k$.
- Trivial vector bundle $T \times \mathbb{C}^k \to \mathbb{C}^k$.
- T_{deg} be the locus of points s.t. $H(t)$ has multiple Eigenvalues. $T_0 := T \setminus T_{deg}$.
- $$\begin{array}{ccccc} T \times \mathbb{C}^k & \hookleftarrow & T_0 \times \mathbb{C}^k & \xrightarrow{\sim} & \bigoplus_{i=1}^k \mathscr{L}_i \\ \downarrow & & \downarrow & \swarrow & \\ T & \hookleftarrow & T_0 & & \end{array}$$

  Need that Eigenvalues are real.
- $c_1(\mathscr{L}_i)$ are the charges corresponding to the Berry phases. Integral over Berry curvature ω [Berry, Simon].
- There are versions for higher degeneracies involving higher Chern–classes. Not today.

Chern classes

2d

If T is two–dimensional compact. Then the Chern classes are given by $\int_T \omega$. This is what happens in the quantum Hall effect. Here $T = T_0 = T^2$. Notice that if $T = T^2$ but $T_{deg} \neq \emptyset$, then all $c_1(\mathscr{L}_i) = 0$. This is the case for graphene $\rightsquigarrow$ Dirac points not topologically protected.

3d

The Chern classes are determined by their pairing with $H_2(T_0, \mathbb{Z})$. If $T = T^3$ there is nice method to encode this using slicing.

Slicing

Setup

- $\pi_i : T^3 = S^1 \times S^1 \times S^1 \to S^1$ the i–th projection.
- $\imath(t) : T^2 = S^1 \times S^1 \to T^3 = S^1 \times S^1 \times S^1$ inclusion $(t_1, t_2) \mapsto (t_1, t_2, t)$.
- $c^i(t) := \int_{T^2} \imath(t)^* c_1(\mathscr{L}_i)$ for $t \notin \pi_3(T_{deg})$.
- For $t \in \pi_3(T_{deg})$ set $c^i(t) := 0$. This is also the result of pulling back the Chern class to $T^2 \setminus \imath(t)^{-1}(T^{deg})$.
- There are of course similar definitions for the other two inclusions and higher dimensions.

Proposition

If T_{deg} is discrete, one can arrange that the $c^i(t)$ for all three projections completely determine the line bundles $\mathscr{L}_i$. (In fact slightly less is needed.)

Chern jumps and local charges

Local charges/jumps

T three dimensional, p isolated point in T_{deg}. The local charges at p are $c^i(p) = \int_{S^2(p)} c_1(\mathscr{L}_i)$ where $S^2(p)$ is a little sphere centered at p.

A local model (Berry, Simons, ...) in 3d for an isolated $2k+1$–dimensional crossing

$H(\mathbf{x}) := \mathbf{x} \cdot \mathbf{L} = xL_x + yL_y + zL_z$ where $L_{x,y,z}$ is a k dimensional representation of spin m.

The local charges are $c^i \in \{-m., \dots, m\}$.

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Jumps for T^3

Assume for convenience that π_3 is locally bijective at p. By Stokes:
$c^i(\pi_3(t_0) + \epsilon) - c^i(\pi_3 - \epsilon) = c^i(p)$
This implies the jumps are in $2\mathbb{Z}$.

Questions

Local models

For a double crossing/Dirac point, the above model is the only model. What are the other local models for higher degeneracies? Phase diagram?

Global properties

1. Depending on properties of $H(t)$ can one say something directly about the $\mathscr{L}_i$ or the c^i?
2. How much does this determine them? Examples: $\sum_i c^i(t) \cong 0$ always. If there is time reversal symmetry $c^i(t) = -c^i(-t)$.
3. How much does knowing the local models determine the global structure?
4. What is the behavior under perturbations?

Our favorite Example, the Gyroid. Newest results

Local Models

The A_1 singularities have the spin local model as needed, but also the A_2 singularities are locally diffeomorphic to the spin 1 case.

Local to global

The local structure of singularities and time reversal symmetry completely determines the functions c^i.

Deformations preserving time reversal symmetry

Numerically, the Dirac points are stable as expected. The A_2 singularities split into four A_1 singularities. This is *a priori* unexpected. *A posteriori* it can be explained as the minimal possible splitting, using the global structure and preserved time reversal symmetry.

Plots

Undeformed case

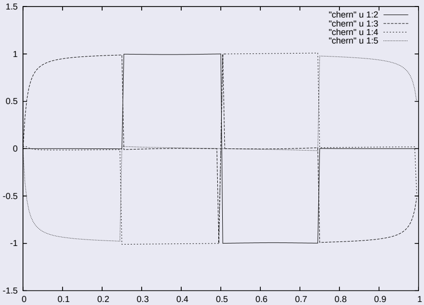


Figure: Slicing along z numerically, can prove anaytically. Corollary: Dirac points in Gyroid are stable

Plots

Deformed case

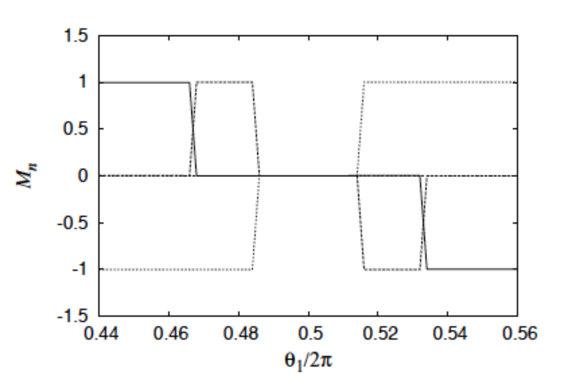


Figure: Slicing along z numerically near the old A_2. This breaks up into *four* A_1 points

Enhanced Symmetries

Re-gauging symmetries

- The graph $\bar{\Gamma}$ has symmetry group $\mathbb{S}_4$.
- This action lifts as regaugings on the Hamiltonians by conjugation of matrices.
- The action can be also be lifted to an action on the torus.
- At points with non–trivial stabilizer groups the matrices above give a projective representation of the stabilizer groups.
- The action of $\mathbb{S}_4$ on T^3 is fixed once we know the action of the generators $(12), (23)$ and (34).
- Both actions can be presented and read off graphically.

Action of $\mathbb{S}_4$ on T^3

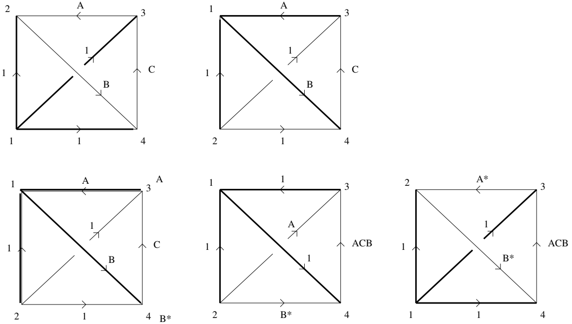


Figure: Calculation of the action of (12) on T^3

$$(A, B, C) \to (A^\star, B^\star, ACB)$$

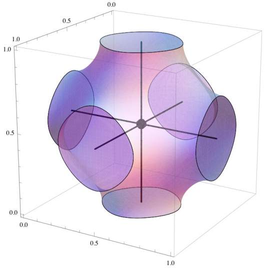
The four degenerate points of the Gyroid

Symmetries at the degenerate points

- The point $(0,0,0)$. The re-gaugeing matrices give the usual representation of $\mathbb{S}_4$ on $\mathbb{C}^4$, decomposing into the trivial representation and an irreducible 3-dim rep. This leads to one three-fold degenerate eigenvalue.
- The point (π,π,π). The re-gaugeing matrices only give a projective representation. We can scale by a 1-cocycle and find again the one-dimensional trivial representation and the 3-dim standard representation.
- The points $(\frac{\pi}{2},\frac{\pi}{2},\frac{\pi}{2})$ and $(\frac{3\pi}{2},\frac{3\pi}{2},\frac{3\pi}{2})$. We have a projective representation of A_4. After scaling by a 1-cocycle, we find a representation of $2A_4$ or binary tetrahedral group. This leads to two eigenvalues with degeneracy 2 (two 2–dim irreps).

The other two cases: P and D

There are only three (families) of triply periodic minimal surfaces whose complements are given by symmetric and self-dual graphs (1) the P or primitive or cubic surface, (2) the D or diamond surface and (3) the G or gyroid surface.



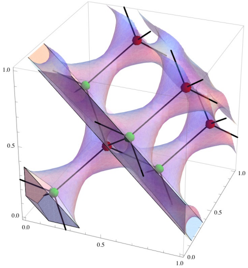


Figure: One channel of the P surface and of the diamond surface and their skeletal graph. The red and green dots refer to the vertices of the two interlaced fcc lattices

The quotient graphs of the surfaces

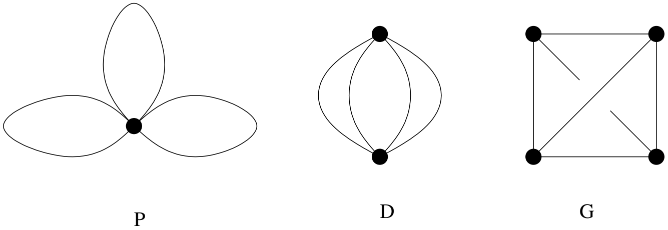


Figure: The quotient graphs for the cubic, diamond and gyroid lattices

Results on P and D

P surface

This is just the case of $\mathbb{Z}^3$. $\mathscr{B}_\Theta = \mathbb{T}^3_\Theta$. There is only one Eigenvalue and hence no degeneracies for $B = 0$.

D surface

The locus where the $\mathscr{B}_\Theta$ is not the full matrix algebra is given by three one dimensional families — again parameterized by the magnetic field parameters. And several special points corresponding to bosonic and fermionic cases.
The locus of degenerate Eigenvalues in the case $B = 0$ is given by three circles which pairwise touch at a point given by the equations $\phi_i = \pi, \phi_j \equiv \phi_k + \pi \mod 2\pi$ with $\{i, j, k\} = \{1, 2, 3\}$.

Summary

1. Gave mathematical setup for new material.
2. Constructed Bellissard–Harper algebra in general (physical) lattice/graph setting.
3. Proved that it embeds into a matrix algebra of a noncommutative torus.
4. Gave a range of trace argument to show that in the rational case there are only finitely many gaps.
5. Gave the commutative geometry when there is no magnetic field as a ramified cover of a torus.
6. Classified the Bellissard–Harper algebras in the case of a Bravais lattice, the honeycomb lattice and the PDG skeletal graphs.
7. Identified points with degenerate Eigenvalues in PDG cases
8. Showed that degeneracies can be explained by a new semi–classical symmetry.

Summary II

To do list

1. Look at spectrum of H with impurities. Pretty much done numerically. Answer: Dirac points stable.
2. Classify level crossing in the spectrum in terms of first Chern classes. Global/local.
3. Define the corresponding quantities (analogs of Hall conductance etc) in non-commutative geometry and give an algebraic/analytic proof of stability.
4. Find a theory for the c/nc duality if it exists.

The end

Thank you!

$A3$ singularity

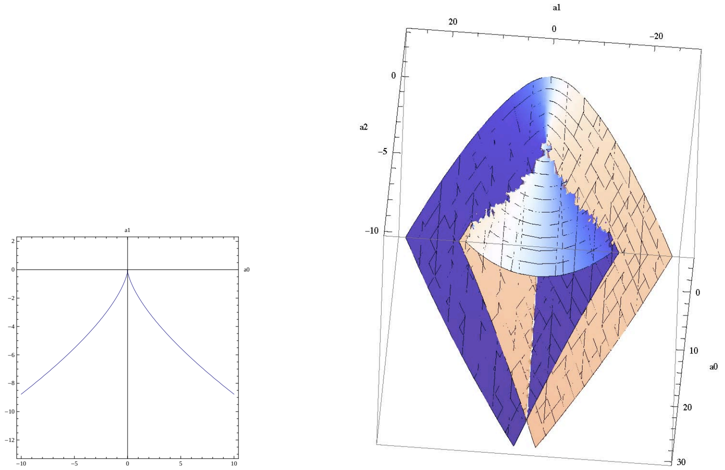


Figure: Disciminant locus in the A_2 and A_3 singularities