Higgs bundles vs Fullerene-like molecules

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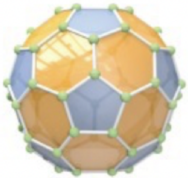
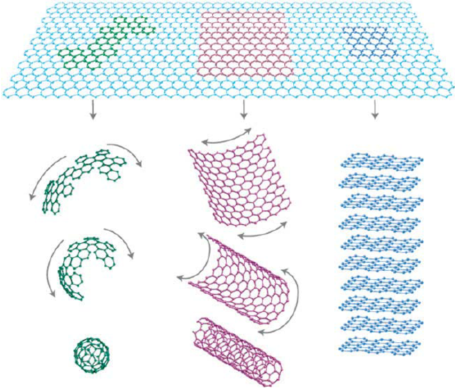
Fullerenes



The Buckminsterfullerene molecule C_{60}

Motivation: Graphene to Fullerene

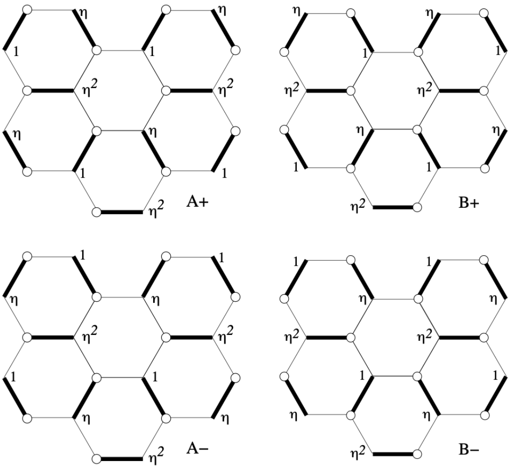


Fullerene Nanotube Graphite

Spherical configurations of graphene are known as fullerenes. The altered topology requires defects where twelve of the regular carbon hexagons are replaced by pentagons.

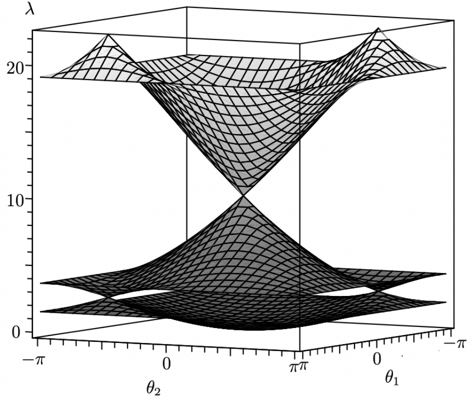
Motivation: Exciting properties of graphene

The electronic properties of graphene are well modelled by a simple Hückel model of nearest-neighbor hopping on a two-dimensional honeycomb lattice:



Motivation: Exciting properties of graphene

Conical singularities



Graphene is expected to exhibit phenomena more familiar in relativistic quantum theory, such as the **Klein Paradox** (unimpeded penetration of relativistic particles through high and wide potential barriers)

Fullerenes: Engel's paper

There are three irreducible fullerenes in the **buckygen** algorithm, isomers of C_{20}, C_{28}, and C_{30}. generates larger fullerenes from smaller ones, by excising a patch of faces and replacing it with a larger patch having the same boundary.

Theorem (Engel, Smillie, '23)

An exact formula for the number of oriented fullerenes with a given number of vertices.

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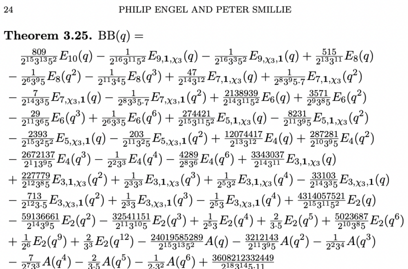
$$BB(q) := \sum_{n \geqslant 1} BB_n q^n =$$
$$q^{10} + q^{12} + q^{13} + 3q^{14} + 3q^{15} + 10q^{16} + 9q^{17} + 23q^{18} +$$

Theorem (Engel, Smillie, '23)

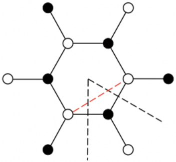
An exact formula for the number of oriented fullerenes with a given number of vertices.



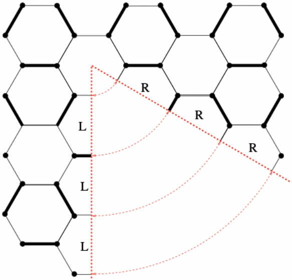
Theorem 3.25. $\mathrm{BB}(q) =$

$$\frac{809}{2^{15}3^{13}5^2}E_{10}(q) - \frac{1}{2^{16}3^{11}5^2}E_{9,\mathbf{1},\chi_3}(q) - \frac{1}{2^{16}3^{3}5^2}E_{9,\chi_3,\mathbf{1}}(q) + \frac{515}{2^{13}3^{11}}E_8(q)$$
$$- \frac{1}{2^{6}3^{9}5}E_8(q^2) - \frac{1}{2^{11}3^{4}5}E_8(q^3) + \frac{47}{2^{14}3^{12}}E_{7,\mathbf{1},\chi_3}(q) + \frac{1}{2^{8}3^{9}5\cdot 7}E_{7,\mathbf{1},\chi_3}(q^2)$$
$$- \frac{7}{2^{14}3^{3}5}E_{7,\chi_3,\mathbf{1}}(q) - \frac{1}{2^{8}3^{3}5\cdot 7}E_{7,\chi_3,\mathbf{1}}(q^2) + \frac{2138939}{2^{14}3^{11}5^2}E_6(q) + \frac{3571}{2^{9}3^{8}5}E_6(q^2)$$
$$- \frac{29}{2^{11}3^{6}5}E_6(q^3) + \frac{1}{2^{6}3^{3}5}E_6(q^6) + \frac{274421}{2^{15}3^{11}5^2}E_{5,\mathbf{1},\chi_3}(q) - \frac{8231}{2^{11}3^{9}5}E_{5,\mathbf{1},\chi_3}(q^2)$$
$$- \frac{2393}{2^{15}3^{2}5^2}E_{5,\chi_3,\mathbf{1}}(q) - \frac{203}{2^{11}3^{2}5}E_{5,\chi_3,\mathbf{1}}(q^2) + \frac{12074417}{2^{13}3^{12}}E_4(q) + \frac{287281}{2^{10}3^{9}5}E_4(q^2)$$
$$- \frac{2672137}{2^{1}13^{9}5}E_4(q^3) - \frac{1}{2^{2}3^{3}}E_4(q^4) - \frac{4289}{2^{8}3^{6}}E_4(q^6) + \frac{3343037}{2^{14}3^{11}}E_{3,\mathbf{1},\chi_3}(q)$$
$$+ \frac{227779}{2^{12}3^{8}5}E_{3,\mathbf{1},\chi_3}(q^2) + \frac{1}{2^{3}3^{3}}E_{3,\mathbf{1},\chi_3}(q^3) + \frac{1}{2^{5}3^{2}}E_{3,\mathbf{1},\chi_3}(q^4) - \frac{33103}{2^{14}3^{3}5}E_{3,\chi_3,\mathbf{1}}(q)$$
$$- \frac{713}{2^{12}3\cdot 5}E_{3,\chi_3,\mathbf{1}}(q^2) + \frac{1}{2^{3}3}E_{3,\chi_3,\mathbf{1}}(q^3) - \frac{1}{2^{5}3}E_{3,\chi_3,\mathbf{1}}(q^4) + \frac{4314057521}{2^{15}3^{11}5^2}E_2(q)$$
$$- \frac{59136661}{2^{14}3^{9}5}E_2(q^2) - \frac{32541151}{2^{11}3^{10}5}E_2(q^3) + \frac{1}{2^{5}3}E_2(q^4) + \frac{2}{3\cdot 5}E_2(q^5) + \frac{5023687}{2^{10}3^{8}5}E_2(q^6)$$
$$+ \frac{1}{2^{6}}E_2(q^9) + \frac{2}{3^{3}}E_2(q^{12}) - \frac{24019585289}{2^{15}3^{13}5^2}A(q) - \frac{3212143}{2^{11}3^{9}5}A(q^2) - \frac{1}{2^{2}3^{4}}A(q^3)$$
$$- \frac{7}{2^{7}3^{3}}A(q^4) - \frac{2}{3\cdot 5}A(q^5) - \frac{1}{2\cdot 3^{2}}A(q^6) + \frac{3608212332449}{2^{18}3^{14}5\cdot 11}$$

Geometric defects: pentagon disclination



The honeycomb lattice comprises of two triangular lattices, A, denoted by black circles and, B, denoted by blank circles. A single pentagonal deformation can be introduced by cutting a $\pi/3$ sector and gluing the opposite sites together.



Higgs bundles

Let Σ be a Riemann surface of genus $g \geqslant 2$ with canonical bundle $K = T^*\Sigma$.

Definition

A Higgs bundle is a pair (E, Φ) for E a holomorphic vector bundle on Σ, and the Higgs field $\Phi \in H^0(\Sigma, End(E) \otimes K)$.

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The field Φ is named by analogy with the Higgs field in physics, which is an additional scalar field "coupled" to other particle fields (i.e. there are terms in Lagrangian involving both the scalar field and other fields). Namely, any time someone adds on an auxilliary field that is coupled to the original data in geometry, they call it a Higgs field.

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Remark: Locally,Φ is a matrix-valued one-form. It has eigenvalues.

Higgs bundles

Each Higgs bundle on Σ will determine a spectral curve $\tilde{\Sigma}$ that forms a branched cover of Σ. Then

$$(E, \Phi) \rightsquigarrow L \text{ on } \tilde{\Sigma}$$

spectral correspondence

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spectral correspondence

Spectral curve is characterized by the coefficients of its characteristic polynomial.

Moduli of Higgs bundles

Therefore, we have Hitchin map:

$$\mathfrak{h}: \ \mathcal{M}^{Higgs} \to \mathcal{B}$$

where $\mathcal{B}$ is the Hitchin base (space of spectral curves).
The remaining spectral data is a line bundle $L \to \tilde{\Sigma}_b$, and for **smooth** $\tilde{\Sigma}_b$, the fiber of the Hitchin map is $Jac(\tilde{\Sigma}_b)$

Remark: $\mathcal{M}^{Higgs}$ inherits a **hyperkähler** structure from the set of pairs (E, Φ). Moreover, the fibers are Lagrangian tori.

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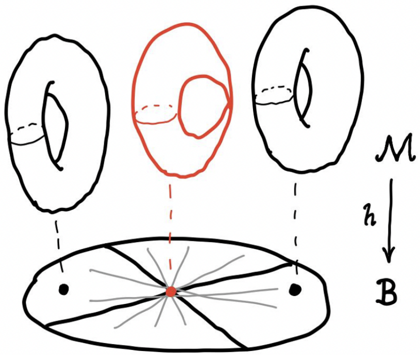


Bloch variety

Crystal momenta are representations of the fundamental group, which all arise from the monodromy of a flat connection, due to the Riemann-Hilbert correspondence:

$$\rho : \pi_1(\Sigma) \to GL(n, \mathbb{C})$$

The Hamiltonian H_ρ for each crystal momentum is defined through the associated Higgs field (E, Φ), via $H_\rho = D_\Phi^* D_\Phi + V$. We can assemble the eigenstates of H_ρ into a master Bloch function $\psi(z, \rho, e)$ satisfying

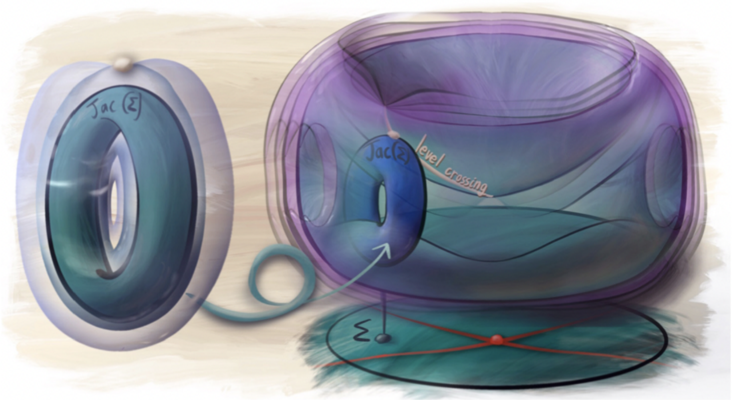
$$H_\rho \psi(z, \rho, e) = e\psi(z, \rho, e)$$

Definition

The band structure is the set of pairs $\rho \in \mathcal{M}^{Higgs}$, $e \in \mathbb{C}$ where the equation has a solution. We call this set the Bloch variety $\beta \subset \mathcal{M}^{Higgs} \times \mathbb{C}$

Remark: This is a codimension 1 analytic **(possibly singular)** submanifold in $\mathcal{M}^{Higgs} \times \mathbb{C}$

Band structure



Credits to E.Kienzle, S. Rayan (Adv.in Math., 2022) for the figure

Each point on the base gives a spectral curve. The Hamiltonian defines a band structure over its fiber, the Jacobian of the spectral curve. These band structures **glue together** to form a master band structure on all $\mathcal{M}^{Higgs}$, represented by the translucent purple shells.

Bloch variety: graphene

Moreover, the level crossings on each fiber glue together to a level crossing set on all $\mathcal{M}^{Higgs}$.

Remark: Level crossings often occur on high-symmetry momenta.

Theorem (Von Neumann-Wigner)

The generic band structures have codimension 2 level crossings.

Therefore, codimension 2 level crossings must be singularities of the Bloch variety

Example:

Dirac points of graphene is an example of conical singularity of the Bloch variety.

Questions (E.Kienzle, S. Rayan (Adv.in Math., 2022)):

1. What is the crystallographic meaning of the principle polarization of the Jacobian or its associated theta divisor?
2. Crystallographic interpretation of the singular fibers?

Tight-binding model

Assumption: A cell only interacts with its neighbors – tightly-bound.

Then the Hamiltonian splits into on-site matrix M and hopping matrices J. The latter couple the cell to its neighbors.
Bloch locus is then the zero set of the characteristic polynomial $\det(H_k - E)$.

Toy model: plane Euclidean crystal

We start with lattice $\Gamma = \langle 1, \tau \rangle \subset \mathbb{C}$, unit cell $\Sigma = \mathbb{C}/\Gamma$ is a genus 1 Riemann surface.
Hamiltonian is $\Delta + V$. Moreover, since the genus is 1 we have $Jac(\Sigma)$ is an elliptic curve. Then a Higgs field with genus 1 spectral curve lives on a rank 2 bundle E over $\mathbb{P}^1$, valued in the line bundle $K(D)$ for a degree 4 divisor D.
The points in D are the roots of degree 4 polynomial $P(z)$, then the Higgs field has determinant proportional to meromorphic quadratic differential

$$\frac{dz^2}{z(z-1)(z-m)}$$

The Hitchin base is $\mathbb{C}$, then the moduli space is a complex surface. And it admits an explicit description.

Fullerenes

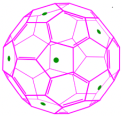
Following the *paper of Kienzle-Rayan*, we assign to each fullerene (for large enough number of atoms) a hyperbolic crystal on $\mathbb{H}$. A crystal structure is given by a discrete group of isometries (Fuchsian group) $\Gamma \subset PSL(2, \mathbb{R})$. By uniformization theorem we know that every Riemann surface Σ with $g \geqslant 2$ is isomorphic to $\mathbb{H}/\Gamma$ for some Γ.

- Γ is isomorphic to $\pi_1(\Sigma)$.

Goal: Band structure for simple fullerenes and how it relates with reality.

Results, '23

For fullerene-like molecules there are six low-lying states that do not depend strongly on the Kekule-induced mass gap.



The coupling configuration of the C_{60} molecule, where vortices reside on the pentagons.

When applied to the leapfrog fullerenes C_{60+6k} it is possible to find that there should be as well six low-lying modes that are insensitive to the magnitude of the Kekule distortion.

Thank you!