Energies and residues of manifolds and configuration space of polygons
Plan of Lectures and Tutorials

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June 2019
Where is Chiba?

We are here

Chiba
What does Chiba mean?

Chiba = 千葉 = thousand leaves = mille feuilles
Purpose and outline of Lectures. The space

- \( X \): a submanifold of \( \mathbb{R}^N \); either
  - \( M^m \): a closed submanifold (\( \partial M = \emptyset \) and \( m < N \))
  - \( \Omega^N \): a compact body (\( = \) the closure of the interior of \( \Omega \))

- We do not consider \( W^m \subset \mathbb{R}^N \) with \( \partial W \neq \emptyset \) and \( m < N \).
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\[\begin{align*}
\text{knot} & \quad \Sigma_2
\end{align*}\]
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![Diagrams](knot.png, \Sigma_2.png, planar domain.png, ball.png)
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![Diagrams](attachment:image.png)
The quantities

- We derive two quantities for $X$ from $\int\int_{X \times X} |x - y|^s \, dx \, dy$

- **Energies**: geometric complexity with information on global shape, e.g., knot energies (cf. KnotPlot by Rob Scharein), generalized Riesz energies

- **Residues**: $\int$ (local quantities), e.g., volume (of $\partial \Omega$), total squared curvature, Willmore functional, (Euler characteristics when $\dim X$ is small)
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Machinery

- Metric (distance function on $X \times X$)

- Start with $I(X, s) := \iint_{X \times X} |x - y|^s \, dx \, dy$

- $I(X, s)$ blows up when $s$ is small ($s \leq -\dim X$)

- Two kinds of regularization from the theory of generalized functions:
  - Hadamard regularization (HR) and
  - regularization via analytic continuation (AC)
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When $s$ is small ($s \leq -\dim X$), $\int\int_{X \times X} |x - y|^s \, dx \, dy$ blows up on the diagonal set $\Delta = \{(x, x) : x \in X\}$.

Consider $\int\int_{X \times X \setminus N_\varepsilon(\Delta)} |x - y|^s \, dx \, dy$ ($\varepsilon > 0$), expand it in a series in $\frac{1}{\varepsilon}$ (a Laurent series of $\varepsilon$)

The constant term is called Hadamard’s finite part, denoted by $\text{Pf.} \int\int_{X \times X} |x - y|^s \, dx \, dy$
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Consider the power $s$ in $\int\int_{X \times X} |x - y|^s \, dx \, dy$ as a complex variable (denoted by $z$ in what follows)

\[ \mathbb{C} \ni z \mapsto \int\int_{X \times X} |x - y|^z \, dx \, dy \in \mathbb{C} \] as a complex function

It is holomorphic when $\Re z$ is big ($\Re z > -\dim X$)

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Energies and residues by two regularizations

- Hadamard regularization.

Laurent series \( p(s; \varepsilon) = \int\int_{X \times X \setminus N_\varepsilon(\Delta)} |x - y|^s \, dxdy \)

- \( s \)-Energy = Pf. \( \int\int_{M \times M} |x - y|^s \, dxdy \), i.e. constant term of \( p(s; \varepsilon) \)

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- Residues are residues of $B_X(z)$
Let us consider some geometric objects in $\mathbb{R}^n$ (usually $n = 2, 3$) such as polygons or (mechanical) linkages (e.g. robot arms). The configuration space (moduli space) is a space of the “shapes”

$$M := \{ \text{geometric objects} \}/G_+,$$

where $G_+$ is the group of the orientation preserving isometries of $\mathbb{R}^n$, $G_+ = SO(n) \rtimes \mathbb{R}^n$.

We study the case when $\dim M$ is finite, especially $\dim M = 1, 2$. 
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We study the case when $\dim \mathcal{M}$ is finite, especially $\dim \mathcal{M} = 1, 2$. 
Example 1: Configuration space of planar pentagons

- E.g.: Config. sp. of pentagons $\subset \mathbb{R}^2$ with fixed edge lengths.
- $(e_1, \ldots, e_5) \in (\mathbb{R}_+)^5$ : given

$$\mathcal{P}(e_1, \ldots, e_5) = \{(P_1, \ldots, P_5) \in (\mathbb{R}^2)^5 : |P_iP_{i-1}| = e_i\}/G_+,$$

- $/G_+$ corresponds to fixing an edge, say $P_1P_2$
- Expected dimension of $\mathcal{P}$: 3 more vertices, 4 more relations (← edge lengths), hence $\dim \mathcal{P} = 3 \times 2 - 4 = 2$
- It is known that when $\mathcal{P}$ is a manifold, i.e., without singularities

$$\mathcal{P} \cong S^2, T^2, \Sigma_2, \Sigma_3, \Sigma_4.$$

The genus can be computed from $(e_1, \ldots, e_5)$
Example 2: Config. sp. of planar “spidery linkages”

Consider mechanical linkages with arms and joints. We assume some of the joints/end points of arms are fixed.

$B_i$ are fixed, located equally on a circle with radius $R$

It can move in the plane

Self-intersection is allowed

Assume $|B_iN_i| = |N_iC| = 1$ ($\forall i$)

$$M \cong \begin{cases} \Sigma_{17} & \text{if } 1 < R < 2 \\ \Sigma_{209} & \text{if } 0 < R < 1 \end{cases}$$
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Study 3D-linkages such that the configuration space is 2 dimensional.
The dimension of the config. sp. of spatial $n$-gons $= 2 \iff n = 4$

Example: $\{3D$-quadrilaterals$\}/G_+ \cong S^2$ or torus or pinched torus

An equilateral and equiangular $n$-gon ($\alpha$-regular stick knot) is a mathematical model of cycloalkane $C_nH_{2n}$.
The dimension of the config. sp. $= 1 \ (n = 6, 7)$ and $= 2 \ (n = 8)$

Dancing hexagons
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**Dancing hexagons**
Equilateral $\arccos(-1/3)$-octagons

Yoshiki Kato did numerical experiments on the case when the bond angle $= \arccos(-1/3)$, the carbon bond angle.

Conjecture (Kato 2019, Master Thesis in Japanese)

$\mathcal{M} \approx$ (homeo. to) a union of two spheres with two points in common (twice pinched torus)
Let $\mathcal{M} = \mathcal{M}(e_1, \ldots, e_8; \theta_1, \ldots, \theta_8)$ be the config. sp. of octagons such that $|P_i - P_{i-1}| = e_i$ and $\angle P_j = \theta_j$.

**Problem**

1. What is the topological type of $\mathcal{M}(1, \ldots, 1; \theta, \ldots, \theta)$?
2. When is $\mathcal{M}(e_1, \ldots, e_8; \theta_1, \ldots, \theta_8)$ a manifold, i.e., without singularities?
3. What are the possible genera of $\mathcal{M}(e_1, \ldots, e_8; \theta_1, \ldots, \theta_8)$?

**Problem**

Can Brylinski’s beta function $B_K(z)$ distinguish points in $\mathcal{M}$? 
Cf. Can you hear the shape of a drum? (Kac)
Brylinski’s beta function of a knot $K$

- $\mathbb{C} \ni z \mapsto \iint_{K \times K} |x - y|^z \, dx \, dy \in \mathbb{C}$ is holomorphic on $\Re z > -1$.

Expand the domain to $\mathbb{C}$ by analytic continuation.

$\leadsto$ a meromorphic function with simple poles at $z = -1, -3, -5, \ldots$.

- It is called Brylinski’s beta function of a knot $K$, denoted by $B_K(z)$.

**Theorem (Brylinski ’99)**

$$B_K(-2) = E(K) = \text{Pf.} \iint_{K \times K} \frac{dxdy}{|x - y|^2}$$

- The residues are geometric quantities of a knot $K$;
  - $\text{Res}(B_K, -1) = 2 \text{Length}(K)$
  - $\text{Res}(B_K, -3) = \frac{1}{4} \int_K \kappa^2 \, dx$

- For the unit circle, $B_\circ(z) = B\left(\frac{z}{2} + \frac{1}{2}, \frac{1}{2}\right)$.
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- $B_K(z)$ has poles at $z = -1, -3, -5, \ldots$ if $K$ is smooth. (The domain depends on the regularity of $K$)

Theorem (Brylinski ’99)

If $K$ is a polygonal knot with $n$ vertices then $B_K(z)$ has simple poles at $z = -1, -2$

- $\text{Res}(B_K, -1) = 2 \text{Length}(K)$

- $\text{Res}(B_K, -2) = -2k + 2 \sum_{j=1}^{n} \frac{\pi - \theta_j}{\sin \theta_j},$

where $\theta_j$ is the angle between adjacent edges.
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*If \( K \) is a polygonal knot with \( n \) vertices then \( B_K(z) \) has simple poles at \( z = -1, -2 \)*

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- \( \text{Res}(B_K, -2) = -2k + 2 \sum_{j=1}^{n} \frac{\pi - \theta_j}{\sin \theta_j} \),

where \( \theta_j \) is the angle between adjacent edges.
Brylinski beta function for polygons

- $B_K(z)$ has poles at $z = -1, -3, -5, \ldots$ if $K$ is smooth. (The domain depends on the regularity of $K$)

Theorem (Brylinski '99)

If $K$ is a polygonal knot with $n$ vertices then $B_K(z)$ has simple poles at $z = -1, -2$

1. $\text{Res}(B_K, -1) = 2 \text{Length}(K)$

2. $\text{Res}(B_K, -2) = -2k + 2 \sum_{j=1}^{n} \frac{\pi - \theta_j}{\sin \theta_j}$,

where $\theta_j$ is the angle between adjacent edges.
Motivation for the energy for knots

Problem (Fukuhara, Sakuma)

Find a functional (which we call an energy) on \{knots\} so that for every knot type we can get an “optimal configuration” as an energy minimizer.
Our strategy

{immersion}
Our strategy

\{non-embedding\}

\{immersion\}
Our strategy

- Each “cell” corresponds to a knot type.
Our strategy

\[
\begin{align*}
&\text{\textit{isotopy class } } [K] \\
&\text{\textit{immersion}} \\
&\text{\textit{non-embedding}}
\end{align*}
\]
Our strategy

- Deform it along the gradient flow of the "energy" $e$. 

![Diagram showing isotopy class $[K]$ and non-embedding, with an arrow pointing to an immersion.]
Our strategy

\[ e([K]) \quad \text{e-minimizer} \quad K_0 \]

\[ e(K_0) = \inf_{K' \in [K]} e(K) =: e[K] \]

\{non-embedding\}

isotopy class \([K]\)

\{immersion\}
Our strategy

- Crossing changes during the deformation process should be avoided!

\[ e([K]) \]

\[ e - \text{minimizer } K_0 \]

\{non-embedding\}

\{immersion\}

\textbf{isotopy class } [K]
We require that our functional $\to +\infty$ as $K$ degenerates to have double points.
Definition of an energy of knots

Definition
A functional $e : \{\text{knots}\} \rightarrow \mathbb{R}$ is called **self-repulsive** if it blows up as a knot degenerates to have double points.

![Diagram of knot degeneration]

Definition
A functional $e : \{\text{knots}\} \rightarrow \mathbb{R}$ is called an **energy** if it is

(i) self-repulsive,
(ii) bounded below,
(iii) continuous in some sense, say w.r.t. $C^2$-top.
**Definition**

A functional \( e : \{\text{knots}\} \to \mathbb{R} \) is called **self-repulsive** if it blows up as a knot degenerates to have double points.

![Diagram showing knot degeneration](image)

**Definition**

A functional \( e : \{\text{knots}\} \to \mathbb{R} \) is called an **energy** if it is

(i) self-repulsive,
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How to get an energy for knots

Candidate: an electrostatic energy of a charged knot

\[ |\text{Coulomb's force}| \propto \frac{1}{r^2}, \text{ potential energy } = \int \int_{K \times K} \frac{dx \, dy}{|x - y|} \]

Apply regularization (HR or AC)
How to get an energy for knots

Candidate: an electrostatic energy of a charged knot

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How to get an energy for knots

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Apply regularization (HR or AC)
Energy of knots

An electrostatic energy of a charged knot
\[ \int \int_{K \times K} \frac{dx \, dy}{|x - y|} \]

Hadamard regularization Pf. \( \int \int_{K \times K} \frac{dx \, dy}{|x - y|} \) is not self-repulsive

Increase the power.
Self-repulsive if the power \( \geq 2 \).

Definition

\[ E(K) := \text{Pf.} \int \int_{K \times K} \frac{dx \, dy}{|x - y|^2} \]
Energy of knots

An electrostatic energy of a charged knot

$$\int\int_{K \times K} \frac{dx \, dy}{|x - y|}$$

Hadamard regularization Pf. \(\int\int_{K \times K} \frac{dx \, dy}{|x - y|}\) is not self-repulsive

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Energy of knots

An electrostatic energy of a charged knot
\[ \iint_{K \times K} \frac{dx \, dy}{|x - y|} \]

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Möbius transformations \(\sim\) inversion in a circle

Inversion in the unit circle of \(\mathbb{C} \cup \{\infty\}\) is given by \(\mathbb{C} \ni z \mapsto \frac{1}{\bar{z}}\).

It is angle-preserving (conformal, i.e. “microscopically homothetic”), and it maps circles (including lines) to circles (including lines).
Möbius transformation

Inversion in a sphere $\Sigma$ with center $C$ and radius $r$

$$P \mapsto \begin{cases} 
\infty & (P = C) \\
C & (P = \infty) \\
P' & (P \neq C, P), \ P' \in \text{half line } CP, \ |CP||CP'| = r^2
\end{cases}$$

A Möbius transformation of $\mathbb{R}^3 \cup \{\infty\}$ is a transformation of $\mathbb{R}^3 \cup \{\infty\}$ that can be obtained as a composition of inversions in spheres (including reflections in planes).
Möbius invariance of the energy of knots

Recall $E(K) = \text{Pf.} \int\int_{K \times K} \frac{dx \ dy}{|x - y|^2}$

Theorem (Freedman-He-Wang '94)

The energy $E$ is invariant under Möbius transformations; $E(T(K)) = E(K)$ for any Möbius transformation $T$ and for any knot $K$.

Corollary

For any prime knot type there is an $E$-minimizer.

prime = not composite

Theorem (Freedman-He-Wang '94)

The round circle gives the minimum value of $E$. 
Energy minimizers by Rob Kusner and John M. Sullivan

Energies and residues of manifolds and configuration space of polygons

Plan of Lectures and Tutorials

June 2019 33 / 34
Related topics

- Regularity of $E$-minimizers. (Zheng-Xu He, Simon Blatt, Philipp Reiter, Armin Schikorra, Aya Ishizeki, Takeyuki Nagasawa, Alexandra Gilsbach, Heiko von der Mosel, and Nicole Vorderobermeier)

- Other energies of knots
- Energy for higher dimensional manifolds (surfaces etc)
- Functionals that measure geometric complexity of mfds.
- Numerical experiments
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