Discretizing Manifolds with Minimal Energy

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Minimization

Questions from physics
• For a system of particles confined to a set $A$ and governed by a pairwise repulsive potential, how does global order (crystalline structure) arise out of energy minimization? That is, what are the ground states of the system?

Generating good node sets
• How to generate a large number of points on a set $A$ that have a uniform or, more generally, a prescribed density with good local properties?
  Sampling for the purpose of quadrature or interpolation, generation of tight frames

Error-correcting codes
• How to maximize separation between a given number of points (words)? Best-packing problems
Energy Kernels

Let \((A, m)\) be an infinite compact metric space.

**Pair Potential** \(K(x, y)\)

\(K : A \times A \to \mathbb{R} \cup \{+\infty\}\) symmetric, lower semi-continuous.

**Popular Potentials:**

Inverse distance kernels: \(K(x, y) = \frac{1}{m(x, y)^s}, \ s > 0\)

Gaussian kernels: \(K(x, y) = \exp(-\alpha m(x, y)^2), \ \alpha > 0\)

\[
\frac{1}{t^s} = \int_0^\infty \exp(-\alpha t^2) \frac{\alpha^{s/2-1}}{\Gamma(s/2)} d\alpha
\]
Discrete Energy

\( K \)-energy of \( \omega_N = \{x_1, \ldots, x_N\} \subset A \) is

\[
E_K(\omega_N) := \sum_{i=1}^{N} \sum_{j=1, j \neq i}^{N} K(x_i, x_j) = \sum_{i \neq j} K(x_i, x_j)
\]

Minimal \( N \)-point \( K \)-energy of the set \( A \) is

\[
\mathcal{E}_K(A, N) := \inf \{ E_K(\omega_N) : \omega_N \subset A, \#\omega_N = N \}.
\]

If \( E_K(\omega_N^*) = \mathcal{E}_K(A, N) \), then \( \omega_N^* \) is called \( N \)-point \( K \)-equilibrium configuration for \( A \) or a set of optimal \( K \)-energy points.

In general, \( \omega_N^* \) is not unique.
Continuous Energy Problem

\( \mathcal{M}(A) \) is set of all probability measures with support on \( A \).

\( K(x, y) \) symmetric, nonnegative, and l.s.c. kernel on \( A \times A \).

**Continuous energy** of \( \mu \in \mathcal{M}(A) \) is defined by

\[
I_K[\mu] := \iint_{A \times A} K(x, y) \, d\mu(x) \, d\mu(y).
\]

**Wiener (Robin) constant** is defined as

\[
W_K(A) := \min \{ I_K[\mu] : \mu \in \mathcal{M}(A) \}.
\]

**Equilibrium measure** is a measure \( \mu_A \in \mathcal{M}(A) \) such that

\[
\]

If \( W_K(A) = \infty \), (i.e. \( \text{cap}_K(A) := 1/W_K(A) = 0 \)), then every \( \mu \in \mathcal{M}(A) \) is an equilibrium measure.
**Fundamental Theorem** (Frostman, Choquet, Fekete, Szegő,...)

With $K$ as above,

\[
\lim_{N \to \infty} \frac{\mathcal{E}_K(A, N)}{N^2} = W_K(A).
\]

Moreover, if $(\omega^*_N)$ is any sequence of $N$-point $K$-energy minimizing configurations on $A$, then every weak* limit measure $\lambda$ as $N \to \infty$ of the normalized counting measures

\[
\nu(\omega^*_N) := \frac{1}{N} \sum_{x \in \omega^*_N} \delta_x
\]

is an equilibrium measure for the continuous energy problem on $A$; i.e., $I_K[\lambda] = W_K(A)$. 
Hereafter $A \subset \mathbb{R}^p$ and $m(x, y) = |x - y|$.

The **Riesz $s$-kernel** is defined by

$$K_s(x, y) := \frac{1}{|x - y|^s}, \quad s > 0; \quad K_{\log}(x, y) := \log\frac{1}{|x - y|}, \quad x, y \in A.$$ 

We write

$$E_s(\omega) := E_{K_s}(\omega), \quad \mathcal{E}_s(A, N) = \mathcal{E}_{K_s}(A, N), \quad s > 0 \text{ or } s = \log.$$ 

For $p = 3$, $s = 1$, get **Coulomb kernel**.

For $A \subset \mathbb{R}^p$ and $s = p - 2$, we get **Newton kernel**.
Best-Packing and Riesz Energy

Separation distance of $\omega_N = \{x_1, \ldots, x_N\} \subset A$

$$\delta(\omega_N) := \min_{1 \leq i \neq j \leq N} |x_i - x_j|.$$ 

$N$-point best-packing distance on $A$,

$$\delta_N(A) := \sup\{\delta(\omega_N) : \omega_N \subset A, \#\omega_N = N\},$$

$\omega_N^*$ is best-packing configuration if $\delta(\omega_N^*) = \delta_N(A)$.

**Proposition: $s \to \infty$ gives best-packing**

For each fixed $N \geq 2$,

$$\lim_{s \to \infty} \mathcal{E}_s(A, N)^{1/s} = \frac{1}{\delta_N(A)}.$$ 

Moreover, every cluster point as $s \to \infty$ of $s$-energy minimizing $N$-point configurations on $A$ is an $N$-point best-packing configuration on $A$. 
What about asymptotics of the minimal energy for $s$ fixed as $N \to \infty$?

What do minimal energy points “look like” for large $N$?
Example: $A = S^2 = \{ x \in \mathbb{R}^3 : |x| = 1 \}$

High precision experiments were conducted to numerically determine $\mathcal{E}_s(S^2, N)$ for $s = \log$, $s = 1$ and $N = 2, 3, \ldots, 200$.

**Bad News:** There are many local minima of energy that are not global minima. Moreover, the local minima have energies very close to $\mathcal{E}_s(S^2, N)$.

**Good News:** Equilibrium points try to distribute themselves over a nearly spherical hexagonal net.
(Local – Global) Energies $4 \leq N \leq 122$
**Good News:** Equilibrium points try to distribute themselves over a ‘nearly’ spherical hexagonal net.

\[ N = 122 \text{ electrons in equilibrium } (s = 1) \]
$N = 1600, s = 4$

Red = heptagon, Green = hexagon, Blue = pentagon
An Example: Torus (Bagel), $N = 1000$
\begin{align*}
\lim_{N \to \infty} \frac{\mathcal{E}_s(A, N)}{N^2} &= W_s(A) = I_s(\mu_A) < \infty, \text{ for } 0 < s < d = \dim_{\mathcal{H}}(A).
\end{align*}

\textbf{“Poppy-Seed Bagel” Theorem (HS (2005) and BHS (2008))}

Suppose \( s \geq d \) and \( A \subset \mathbb{R}^p \) is a \textit{d-rectifiable set} (i.e. Lipschitz image of a compact set in \( \mathbb{R}^d \)). When \( s = d \) we further assume \( A \) is a subset of a \( d \)-dimensional \( C^1 \) manifold. Then

\begin{align*}
\lim_{N \to \infty} \frac{\mathcal{E}_d(A, N)}{N^2 \log N} &= \frac{\mathcal{H}_d(B_d(0, 1))}{\mathcal{H}_d(A)}, \\
\lim_{N \to \infty} \frac{\mathcal{E}_s(A, N)}{N^{1+s/d}} &= \frac{C_{s,d}}{[\mathcal{H}_d(A)]^{s/d}}, \quad s > d.
\end{align*}

where \( C_{s,d} \) does not depend on \( A \) and \( \mathcal{H}_d(\cdot) \) is \( d \)-dim Hausdorff measure.

Further, if \( \mathcal{H}_d(A) > 0 \), optimal \( s \)-energy configurations for \( s \geq d \) are asymptotically (as \( N \to \infty \)) \textbf{uniformly distributed} on \( A \) with respect to \( \mathcal{H}_d \).
"Poppy-Seed Bagel" Theorem, continued

If $\{\omega_N^*\}_{N=2}^\infty$ is a sequence of minimal $s$-energy configurations on the $d$-rectifiable set $A$ with $s > d$, then the sequence has "optimal order separation"; i.e.,

$$\delta(\omega_N^*) \asymp \frac{1}{N^{1/d}}, \quad N \to \infty.$$  

Furthermore, if $A$ is also $d$-regular, then the sequence $\{\omega_N^*\}$ provides "optimal order covering"; i.e.,

$$\rho(\omega_N^*, A) := \max_{y \in A} \min_{x \in \omega_N^*} |y - x| \asymp \frac{1}{N^{1/d}}, \quad N \to \infty.$$  

By "$d$-regular" we mean there is a positive measure $\mu$ supported on $A$ and $c_1, c_2 > 0$ such that

$$c_1 r^d \leq \mu(B(x, r)) \leq c_2 r^d, \quad x \in A, \ 0 < r < \text{diam}(A).$$
An Example: Torus (Bagel), $N = 1000$
What is this mysterious constant constant \( C_{s,d} \) ?

\( d=1: \) (M-F, M, R,S)

From optimality of the roots of unity on \( S^1 \),

\[
C_{s,1} = 2\zeta(s) \quad \text{for} \quad s > 1,
\]

where \( \zeta(s) = \sum_{k=1}^{\infty} 1/k^s \) is the classical Riemann zeta function.

For other fixed dimensions \( d \) is \( C_{s,d} \) some type of generalized "zeta function" of \( s \) ?
The $d$-dimensional packing density $\Delta_d$ is the maximum fraction of the space $\mathbb{R}^d$ that can be covered by a collection of non-overlapping balls of the same radius.

Connection between $C_{s,d}$ and $\Delta_d$ (Bor, Har, S):

$$(C_{s,d})^{1/s} \to (1/2) \left( \frac{\text{Vol}(B_d(0, 1))}{\Delta_d} \right)^{1/d} \text{ as } s \to \infty$$

$\Delta_1 = 1,$

$\Delta_2 = \pi/\sqrt{12}$ (Fejes-Toth, 1940), hexagonal lattice

$\Delta_3 = \pi/\sqrt{18}$ (Kepler Conjecture proved by Hales, 2005), FCC lattice

$\Delta_8 = \pi^4/384$ (Viazovska, 2017), $E_8$ lattice

$\Delta_{24} = \pi^{12}/12! \approx 0.002$ (Co,Ku,Mi,Ra,Vi, 2017), Leech lattice
Upper Bounds for $C_{s,d}$

Let $\Lambda$ denote a lattice of rank $d$ in $\mathbb{R}^d$, that is, $\Lambda = V\mathbb{Z}^d$, where $V$ is a $d \times d$ matrix of full rank.

**Epstein Zeta Function**

$$\zeta_{\Lambda}(s) := \sum_{v \in \Lambda, v \neq 0} \frac{1}{|v|^s}, \ s > d.$$ 

**Proposition**

$$C_{s,d} \leq \min_{\Lambda} |\Lambda|^{s/d} \zeta_{\Lambda}(s), \ s > d,$$

where the min is taken of all lattices of rank $d$ and $|\Lambda|$ is the co-volume of the lattice.
Proof of Proposition

Let $\Omega = \Omega_\Lambda$ denote a fundamental polytope for $\Lambda$. For $m \in \mathbb{N}$, put $X_m := \Omega \cap \frac{1}{m} \Lambda$. Then $|X_m| = m^d =: N$ and

$$E_s(X_m) = \sum_{x \in X_m} \sum_{y \in X_m, y \neq x} |x - y|^{-s} \leq N \sum_{y \in \frac{1}{m} \Lambda, y \neq x_m \in X_m} |x_m - y|^{-s}$$

$$\leq N \sum_{v \in \Lambda, v \neq v_m \in \Lambda} \left| \frac{1}{m} v_m - \frac{1}{m} v \right|^{-s} = N \cdot m^s \sum_{v \in \Lambda, v \neq v_m} |v_m - v|^{-s} = N^{1+s/d} \zeta_\Lambda(s).$$

$$\frac{E_s(\Omega, N)}{N^{1+s/d}} \leq \frac{E_s(X_m)}{N^{1+s/d}} \leq \zeta_\Lambda(s)$$

Let $m \to \infty$ ($N \to \infty$),

$$\frac{C_{s,d}}{|\Lambda|^{s/d}} \leq \zeta_\Lambda(s).$$
Conjectures for the Constant $C_{s,d}$

For $d = 2, 4, 8, \text{ and } 24$,

$$C_{s,d} = |\Lambda|^{s/d} \zeta_\Lambda(s), \quad s > d,$$

where $\Lambda$ is, respectively, the hexagonal, $D_4$, $E_8$, and Leech lattice.

Kuijlaars-S Conjecture, 1998

\[ C_{s,2} = \left(\frac{\sqrt{3}}{2}\right)^{s/2} \zeta_\Lambda(s), \quad s > 2, \]

where $\zeta_\Lambda := \sum_{0 \neq \mathbf{v} \in \Lambda} |\mathbf{v}|^{-s}$,

$\Lambda = \{k_1 \mathbf{v}_1 + k_2 \mathbf{v}_2 : k_1, k_2 \in \mathbb{Z}\}.$
Lower Bound for $C_{s,d}$

**Theorem** (HarMicSaf, 2018)

For a fixed dimension $d$, let $z_1 < z_2 < \cdots$ be the positive roots of the Bessel function $J_{d/2}(z)$. Then, for $s > d$,

$$C_{s,d} \geq A_{s,d},$$

where

$$A_{s,d} := \left[ \frac{\pi^{d+1/2} \Gamma(d+1)}{\Gamma(d+1/2)} \right]^{s/d} \frac{4}{\lambda_d \Gamma(d+1)} \sum_{i=1}^{\infty} (z_i)^{d-s-2} (J_{d/2+1}(z_i))^{-2}$$

and $\lambda_d := \sqrt{\pi} \Gamma(d/2)/\Gamma(d+1/2)$.

For $d = 1$, $A_{s,d} = 2\zeta(s)$, which is optimal.

**Corollary**

For every fixed $d \geq 1$, $C_{s,d}$ has a simple pole at $s = d$ with residue

$$\lim_{s \to d^+} (s - d) C_{s,d} = \frac{2\pi^{d/2}}{\Gamma(d/2)}.$$
Graphs of \((C_{s,d}^{(\text{conj})}/A_{s,d})^{1/s}\) for \(d = 2, 4, 8\) and 24.
Not the Perfect Poppy-Seed Bagel
How to get our lower bound? LP on the sphere

- Spherical Code: A finite set $C \subset S^{n-1} \subset \mathbb{R}^n$ with cardinality $|C|$;
- For $x, y \in S^{n-1}$, $|x - y|^2 = 2 - 2\langle x, y \rangle$;
- $K(x, y) = h(t)$, $t = \langle x, y \rangle$, where $h: [-1, 1] \to \mathbb{R} \cup \{+\infty\}$ is an absolutely monotone\(^1\) function;
- Riesz $s$-potential: $h(t) = (2 - 2t)^{-s/2} = |x - y|^{-s}$

The $h$-energy of a spherical code $C$:

$$E_K(C) = E(n, C; h) := \sum_{x, y \in C, x \neq y} h(\langle x, y \rangle).$$

- $\mathcal{E}(n, N, h) := \min_{|C| = N} E(n, C; h)$.

\(^1\)A function $f$ is absolutely monotone on $I$ if $f^{(k)}(t) \geq 0$ for $t \in I$ and $k = 0, 1, 2, \ldots$.
Spherical Harmonics and Gegenbauer polynomials

- **Harm**$(k)$: homogeneous harmonic polynomials in $n$ variables of degree $k$ restricted to $S^{n-1}$. Then

  $$r_{k,n} := \dim \text{Harm}(k) = \binom{k + n - 3}{n - 2} \binom{2k + n - 2}{k}.$$  

- **Spherical harmonics** (degree $k$): \{ $Y_{kj}(x) : j = 1, 2, \ldots, r_{k,n}$ \} orthonormal basis of $\text{Harm}(k)$ with respect to normalized $(n - 1)$-dimensional surface area measure on $S^{n-1}$.

- **Gegenbauer polynomials** $P^{(n)}_k(t)$ associated with $S^{n-1}$ are special types of **Jacobi polynomials** $P^{(\alpha,\beta)}_k(t)$ orthogonal on $[-1, 1]$ w.r.t. weight $(1 - t)^\alpha (1 + t)^\beta$, where $\alpha = \beta = (n - 3)/2$. We use the normalization $P^{(n)}_k(1) = 1$ for all degrees $k$. 

Spherical Harmonics and Gegenbauer polynomials

• The Gegenbauer polynomials and spherical harmonics are related through the well-known **Addition Formula**:

\[
\sum_{j=1}^{r_{k,n}} Y_{kj}(x) Y_{kj}(y) = r_{k,n} P_k^{(n)}(t), \quad t = \langle x, y \rangle, \ x, y \in S^{n-1}.
\]

• **Consequence:** If \( C \) is a spherical code of \( N \) points on \( S^{n-1} \),

\[
\sum_{x,y \in C} P_k^{(n)}(\langle x, y \rangle) = \frac{1}{r_{k,n}} \sum_{j=1}^{r_{k,n}} \sum_{x \in C} \sum_{y \in C} Y_{kj}(x) Y_{kj}(y)
\]

\[
= \frac{1}{r_{k,n}} \sum_{j=1}^{r_{k,n}} \left( \sum_{x \in C} Y_{kj}(x) \right)^2 \geq 0.
\]
‘Good’ potentials for lower bounds - Delsarte-Yudin LP

Delsarte-Yudin approach:

Find a potential $f$ such that $h \geq f$ for which we can obtain good lower bounds for the minimal $f$-energy $\mathcal{E}(n, N; f)$.

Suppose $f : [-1, 1] \to \mathbb{R}$ is of the form

$$f(t) = \sum_{k=0}^{\infty} f_k P_k^{(n)}(t), \quad f_k \geq 0 \text{ for all } k \geq 1, \quad f(1) < \infty.$$  

Then for $C \subset S^{n-1}$, $|C| = N$,

$$E(n, C; f) = \sum_{x, y \in C, x \neq y} f(\langle x, y \rangle) = \sum_{x, y \in C} f(\langle x, y \rangle) - f(1)N$$

$$= \sum_{k=0}^{\infty} f_k \sum_{x, y \in C} P_k^{(n)}(\langle x, y \rangle) - f(1)N$$

$$\geq f_0 N^2 - f(1)N = N^2 \left(f_0 - \frac{f(1)}{N}\right).$$
Thm (Delsarte-Yudin LP Bound)

Let $A_{n,h} := \{ f : f(t) \leq h(t), \, t \in [-1, 1], \, f_k \geq 0, \, k = 1, 2, \ldots \}$. Then

$$\mathcal{E}(n, N; h) \geq \mathcal{E}(n, N; f) \geq N^2 \left( f_0 - \frac{f(1)}{N} \right), \quad f \in A_{n,h}. \quad (1)$$
Thm (Delsarte-Yudin LP Bound)

Let \( A_{n,h} := \{ f : f(t) \leq h(t), t \in [-1, 1], \ f_k \geq 0, \ k = 1, 2, \ldots \} \). Then

\[
\mathcal{E}(n, N; h) \geq \mathcal{E}(n, N; f) \geq N^2 \left( f_0 - \frac{f(1)}{N} \right), \quad f \in A_{n,h}.
\] (1)

The full LP problem consists of maximizing the lower bound, that is, the linear objective functional,

\[
F(f) := N^2 \left( f_0 - \frac{f(1)}{N} \right),
\]

over all continuous \( f \) subject to \( f \in A_{n,h} \).
Thm (Delsarte-Yudin LP Bound)

Let $A_{n,h} := \{ f : f(t) \leq h(t), t \in [-1, 1], f_k \geq 0, k = 1, 2, \ldots \}$. Then

$$E(n, N; h) \geq E(n, N; f) \geq N^2 \left( f_0 - \frac{f(1)}{N} \right), \quad f \in A_{n,h}. \quad (1)$$

Full linear programming is too ambitious, truncate to a finite dimensional LP problem by maximizing

$$F(f) := N^2 \left( f_0 - \frac{f(1)}{N} \right),$$

subject to $f \in \mathcal{P}_m \cap A_{n,h}$, with $\mathcal{P}_m$ denoting all polynomials of deg $\leq m$. 
Lower Bounds and 1/N-Quadrature Rules

Definition

For a subspace $\Lambda \subset C([-1,1])$ and $N > 1$, we say $\{(\alpha_i, \rho_i)\}_{i=1}^k$ is a 1/N-quadrature rule exact for $P_m$ if $-1 \leq \alpha_i < 1$ and $\rho_i > 0$ for $i = 1, 2, \ldots, k$ if for all $f \in P_m$,

$$f_0 = \gamma_n \int_{-1}^{1} f(t)(1 - t^2)^{(n-3)/2} dt = \frac{f(1)}{N} + \sum_{i=1}^{k} \rho_i f(\alpha_i).$$

Thus for $f \in P_m \cap A_{n,h}$,

$$\varepsilon(n, N; h) \geq N^2 \left( f_0 - \frac{f(1)}{N} \right) = N^2 \sum_{i=1}^{k} \rho_i f(\alpha_i).$$

whenever such a quadrature rule exists.
Where to find such $1/N$ quadrature rules?

Spherical Designs

Levenshtein’s Framework for Maximal Codes
Spherical Designs and DGS Bound


**Definition**

A **spherical** $\tau$-**design** $C \subset S^{n-1}$ is a finite nonempty subset of $S^{n-1}$ such that

$$
\frac{1}{\sigma(S^{n-1})} \int_{S^{n-1}} p(x) \, d\sigma(x) = \frac{1}{|C|} \sum_{x \in C} p(x)
$$

($\sigma(x)$ is surface area measure on $S^{n-1}$) holds for all polynomials $p(x) = p(x_1, x_2, \ldots, x_n)$ of degree at most $\tau$.

The **strength** of $C$ is the maximal number $\tau = \tau(C)$ such that $C$ is a spherical $\tau$-design.
Spherical Designs and DGS Bound


**Definition**

A **spherical τ-design** $C \subset S^{n-1}$ is a finite nonempty subset of $S^{n-1}$ such that

$$\frac{1}{\sigma(S^{n-1})} \int_{S^{n-1}} p(x) \, d\sigma(x) = \frac{1}{|C|} \sum_{x \in C} p(x)$$

($\sigma(x)$ is surface area measure on $S^{n-1}$) holds for all polynomials $p(x) = p(x_1, x_2, \ldots, x_n)$ of degree at most $\tau$.

The **strength** of $C$ is the maximal number $\tau = \tau(C)$ such that $C$ is a spherical $\tau$-design.
What is minimum number of points needed for a $\tau$-design?

**Theorem (DGS - 1977)**

For fixed strength $\tau$ and dimension $n$ denote by

$$B(n, \tau) := \min \{|C| : \exists \text{ } \tau\text{-design } C \subset S^{n-1}\}$$

the minimum possible cardinality of spherical $\tau$-designs $C \subset S^{n-1}$.

$$B(n, \tau) \geq DGS(n, \tau) := \begin{cases} 
2\binom{n+k-2}{n-1}, & \text{if } \tau = 2k - 1, \\
\binom{n+k-1}{n-1} + \binom{n+k-2}{n-1}, & \text{if } \tau = 2k.
\end{cases}$$
1/N-Quadrature Rules

Quadrature Rules from Spherical Designs

If $C \subset S^{n-1}$ is a spherical $\tau$ design and $\Lambda = \mathcal{P}_\tau$, then choosing
\[ \{\alpha_1, \ldots, \alpha_k, 1\} = \{\langle x, y \rangle : x, y \in C\} \] and $\rho_i =$ fraction of times $\alpha_i$ occurs in $\{\langle x, y \rangle : x, y \in C\}$ gives a $1/N$ quadrature rule exact for $\Lambda$.

This follows from the fact that for a $\tau$-design $C$,
\[ \sum_{x,y \in C} P_k^{(n)}(\langle x, y \rangle) = \frac{1}{r_{k,n}} \sum_{j=1}^{r_{k,n}} \left( \sum_{x \in C} Y_{kj}(x) \right)^2 = 0, \text{ for } 1 \leq k \leq \tau \]
and so if $f \in \mathcal{P}_\tau$, then
\[ \sum_{x,y \in C} f(\langle x, y \rangle) = \sum_{k=0}^{\tau} \sum_{x,y \in C} f_k P_k^{(n)}(\langle x, y \rangle) = N^2 f_0, \]

\[ f_0 = \frac{1}{N^2} \sum_{x,y \in C} f(\langle x, y \rangle) = \frac{1}{N} f(1) + \sum_{i=1}^{k} \rho_i f(\alpha_i). \]
Sharp Codes

**Definition**

A spherical code $C \subset \mathbb{S}^{n-1}$ is a *sharp* if there are exactly $m$ inner products between distinct points in it and it is a spherical $(2m - 1)$-design.

**Theorem (Cohn and Kumar, 2007)**

If $C \subset \mathbb{S}^{n-1}$ is a sharp code as above, then $C$ is universally optimal; i.e., $C$ is $h$-energy optimal for any $h$ that is absolutely monotone on $[-1, 1]$.

**Theorem (Cohn and Kumar, 2007)**

Let $C$ be the 600-cell (120 in $\mathbb{R}^4$). Then there is $f \in \Lambda \cap A_{4,h}$, s.t. $f(\langle x, y \rangle) = h(\langle x, y \rangle)$ for all $x \neq y \in C$, where

$\Lambda = \mathcal{P}_{17} \cap \{f_{11} = f_{12} = f_{13} = 0\}$. Hence it is a universal code.
Levenshtein $1/N$-Quadrature Rule - odd order case

- For every fixed $N \geq \text{DGS}(n, 2k - 1) := 2 \binom{n + k - 2}{n - 1}$ there exist uniquely determined real numbers $-1 \leq \alpha_1 < \alpha_2 < \cdots < \alpha_k < 1$ and positive weights $\rho_1, \rho_2, \ldots, \rho_k$ such that the equality

$$f_0 = \frac{f(1)}{N} + \sum_{i=1}^{k} \rho_i f(\alpha_i)$$

holds for every polynomial $f(t)$ of degree at most $2k - 1$.

- The numbers $\alpha_i, i = 1, 2, \ldots, k$, are the roots of the equation

$$P_k(t)P_{k-1}(s) - P_k(s)P_{k-1}(t) = 0,$$

where $s = \alpha_k$, $P_i(t) = P^{(n-1)/2,(n-3)/2}_i(t)$ is a Jacobi polynomial.
Universal Lower Bound, ULB

Theorem - (BDHSS - Constr. Approx.)

Let $h$ be absolutely monotone, $n, k$ and $N$ be such that $N \geq \text{DGS}(n, 2k - 1)$. Then for the Levenshtein $1/N$-QR\{$(\alpha_i, \rho_i)$\}$_{i=1}^{k}$ for $\mathcal{P}_{2k-1}$,

$$\mathcal{E}(n, N, h) \geq N^2 \sum_{i=1}^{k} \rho_i h(\alpha_i).$$

Moreover, the Hermite interpolants at these nodes are the optimal polynomials that solve the finite LP in the class $\mathcal{P}_{2k-1} \cap A_{n,h}$.

Similar result holds for $\mathcal{P}_{2k} \cap A_{n,h}$. 
Sketch of the proof of ULB theorem

• Let $f(t)$ be the Hermite interpolant of degree $m = 2k - 1$ s.t.

$$f(\alpha_i) = h(\alpha_i), \ f'(\alpha_i) = h'(\alpha_i), \ i = 1, 2, \ldots, k;$$

• The absolute monotonicity implies $f(t) \leq h(t)$ on $[-1, 1]$;

• The Hermite interpolant at the $\alpha_i$’s has positive Gegenbauer coefficients (using methods from Cohn-Kumar, 2007). So,

$$f(t) \in \mathcal{P}_m \cap A_{n,h}.$$
Gaussian energy comparison (BBCGKS 2006) - $N = 5$ – 64, $n = 4$. 
Proof of Lower Bound for $C_{s,d}$

Take $N = N_k := \text{DGS}(n, 2k - 1)$ and apply the ULB result to $h(t) = (2 - 2t)^{-s/2}$.

For this we need asymptotics for Levenshtein nodes $\alpha_i = \alpha^{(N)}_i$ and the weights $\rho_i = \rho^{(N)}_i$ as $N \to \infty$.

**Lemma : Connection with Bessel Functions**

Let $-1 < \gamma_{k,k} < \cdots < \gamma_{k,1} < 1$ be the zeros of $P^{(\alpha,\beta)}_k(t)$, and denote by $z_i$ the $i$-th smallest positive zero of the Bessel function $J_\alpha(z)$. Then for all $i = 1, 2, \ldots$, 

$$
\lim_{k \to \infty} kP^{(\alpha,\beta)}_{k-1}(\gamma_{k,i}) = 2\Gamma(\alpha + 1) \left( \frac{z_i}{2} \right)^{-\alpha+1} J_{\alpha+1}(z_i).
$$
Energy of Configurations in $\mathbb{R}^d$

**Definition**

For an infinite configuration $C \subset \mathbb{R}^d$ and $f : (0, \infty) \to \mathbb{R}$ of rapid decay, the *f-energy of $C$* is

$$E_f(C) := \lim_{r \to \infty} \frac{1}{\#(C \cap B_d(0, r))} \sum_{\substack{x, y \in C \cap B_d(0, r) \\ x \neq y}} f(|x - y|),$$

provided the limit exists. Here $B_d(0, r)$ is the $d$-dimensional ball of radius $r$ centered at 0.

**Definition**

The *density* $\rho$ of a configuration $C$ is defined to be

$$\rho := \lim_{r \to \infty} \frac{\#(C \cap B_d(0, r))}{\text{vol}(B_d(0, r))},$$

provided this limit exists.
Lower Bound for Gaussian Energy

**Theorem** (Cohn, de Courcy Ireland), (HarMicSaf)

Let $f(|x - y|) = e^{-\alpha |x-y|^2}$, $\alpha > 0$, be a **Gaussian potential** in $\mathbb{R}^d$ and choose $R$ so that $\text{vol}(B_d(0, R/2)) = \rho$. Then the minimal $f$-energy for point configurations of density $\rho$ in $\mathbb{R}^d$ is bounded below by

$$
\frac{4}{\lambda_d \Gamma(d + 1)} \sum_{i=1}^{\infty} \frac{z_i^{d-2}}{J_{d/2+1}(z_i)} f\left(\frac{Z_i}{\pi R}\right),
$$

where the $z_i$’s are as in the lower estimate for $C_{s,d}$.

Here we need to go from estimates on the sphere $S^d$ for

$$
f_N(|x - y|) = h_N(\langle x, y \rangle) := e^{-\alpha \frac{2 - 2 \langle x, y \rangle}{(cN^{-1/d})^2}}.
$$

to estimates for the Gaussian potential in $\mathbb{R}^d$. 
Graphs of $(\tilde{C}_{s,d}/A_{s,d})^{1/s}$ for $d = 2, 4, 8$ and 24.
Minimal Riesz $s$-Energy for $N = 5$ on $S^2$
Minimal Riesz $s$-Energy for $N = 5$ on $S^2$

bipyramid

square-base pyramid
Minimal Riesz $s$-Energy for $N = 5$ on $S^2$

**Ratio** of $s$-energy of **bipyramid** to $s$-energy of **optimal sq-base pyramid**

Melnyk et al (1977) Bipyramid appears optimal for $0 < s < s^*$ where $s^* \approx 15.04808$.

Recently proved by R. Schwartz (over 150 pages + computer assist). **Open problem for** $s > s^* + \epsilon$
Minimal Riesz $s$-Energy for $N = 5$ on $S^2$

**Ratio** of $s$-energy of **bipyramid** to $s$-energy of **optimal sq-base pyramid**

Melnyk et al (1977) **Bipyramid appears optimal for $s$ up to $s \approx 15$**

P. Dragnev et al. $s = \log$, R. Schwartz $0 < s \leq 6$
MORALS

Optimal Riesz $s$-energy configurations, in general, depend on $s$.

Rigorous proofs of computational observations can be quite difficult.