Universal optimality of the E_8 and Leech lattices

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Arranging points in Euclidean spaces

Question

What is the best way to arrange a discrete set of points in $\mathbb{R}^d$?

The answer depends on the objective:

- Symmetries
- Separation properties
- Sampling/interpolation
- etc.

Imagine a collection of particles that repel each other.
Stable equilibrium: minimize the potential energy among all configurations $\mathcal{C} \subset \mathbb{R}^d$

$$\min_{\mathcal{C}} \sum_{x,y \in \mathcal{C}} g(|x-y|)$$

Energy minimization in Euclidean spaces

Definition

Let $p\colon (0,\infty) \to \mathbb{R}$ be a bounded nonnegative function. For a discrete configuration $\mathcal{C} \subset \mathbb{R}^d$ we define its p-energy as

$$E_p(\mathcal{C}) = \liminf_{R\to\infty} \frac{1}{|\mathcal{C} \cap B_R|} \sum_{\substack{x\neq y \\ x,y\in\mathcal{C}\cap B_R}} p(|x-y|^2).$$

Definition

Density of $\mathcal{C}$ is given by

$$\rho(\mathcal{C}) = \lim_{R\to\infty} \frac{|\mathcal{C} \cap B_R|}{Vol(B_R)}$$

Energy minimization in Euclidean spaces

Problem

Given a potential p find the minimum (infimum) of $E_p(\mathcal{C})$ among all configurations $\mathcal{C} \subset \mathbb{R}^d$ with density ρ. Describe all $\mathcal{C} \subset \mathbb{R}^d$ of density ρ that achieve this minimum.

This is much, much harder than it might sound.

Important potentials

- Hard ball potential

$$p(r) = \begin{cases} 1\,, & r < 4R^2 \\ 0\,, & r \geq 4R^2 \end{cases}$$

- Riesz potential

$$p(r) = r^{-s} \qquad s > 0$$

- Gaussian potential (Gaussian core model)

$$p(r) = \exp(-\alpha\pi r) \qquad \alpha > 0$$

The last two potentials are completely monotone: $(-1)^k p^{(k)}(r) > 0$, $k \geq 0$.

Important potentials

The p-energy of lattices arises naturally in number theory.

If $p(r) = e^{-\alpha\pi r}$ then

$$E_p(\Lambda) = \sum_{x \in \Lambda \setminus \{0\}} e^{-\alpha\pi|x|^2} = \Theta_\Lambda(i\alpha) - 1$$

If $p(r) = r^{-s}$ and $s > d/2$ then

$$E_p(\Lambda) = \sum_{x \in \Lambda \setminus \{0\}} |x|^{-2s} = \zeta_\Lambda(s)$$

Sphere packing

When $p(r)$ is the hard ball potential, minimizing $E_p(\mathcal{C})$ is the sphere packing problem.

- Density:

$$\rho(\mathcal{C}) = \lim_{R\to\infty} \frac{|\mathcal{C} \cap B_R|}{Vol(B_R)}$$

- Packing distance:

$$R(\mathcal{C}) = \min_{\substack{x,y\in\mathcal{C}\\ x\neq y}} |x-y|$$

Problem (Sphere packing problem, Kepler problem)

What is the maximum packing distance among configurations of fixed density in $\mathbb{R}^d$.

Energy minimization and sphere packing

Sphere packing and other energy minimization problems are closely related.

Proposition

If $\mathcal{C}$ is optimal for Riesz potential $p(r) = r^{-s}$ for all sufficiently large $s > 0$, then $\mathcal{C}$ is an optimal sphere packing.

Proposition

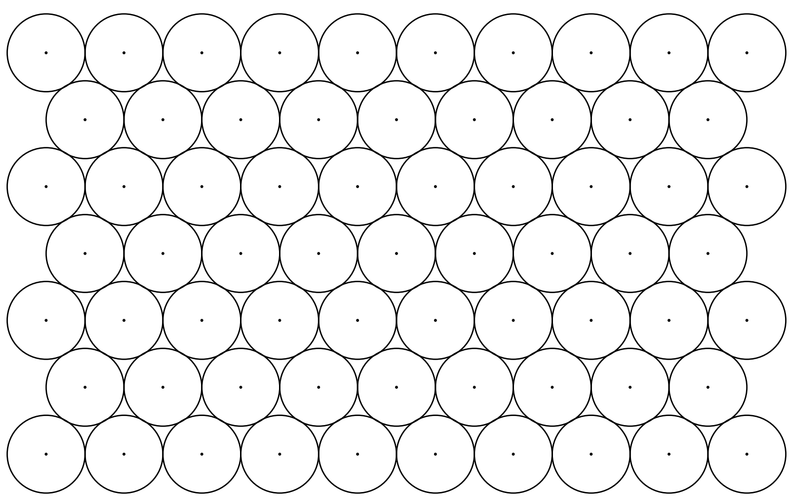
If $\mathcal{C}$ is optimal for the Gaussian potential $p(r) = e^{-\alpha\pi r}$ for all sufficiently large $\alpha > 0$, then $\mathcal{C}$ is an optimal sphere packing.

Known results for sphere packing

d	$\mathcal{C}$	Proof
1	$\mathbb{Z}$	Trivial
2	A_2	Thue (1890), Fejes Tóth (1940)
3	$fcc, hcp, \ldots$	Hales (1998/2014)
4	D_4?	Open problem
5	D_5?	Open problem
6	E_6?	Open problem
7	E_7?	Open problem
8	E_8	Viazovska (2016)
24	Λ_{24}	Cohn-Kumar-Miller-R.-Viazovska (2016)

Two-dimensional case

Optimal sphere packing in two-dimensions (hexagonal lattice A_2)



Two-dimensional case

That A_2 is the best sphere packing was rigorously proved by Fejes Tóth in 1940.

Conjecture

A_2 is optimal for Riesz potentials $p(r) = r^{-s}$ for all $s > 1$.

This is not known for any single value of s!

Theorem (Montgomery)

A_2 is optimal for Riesz potentials among lattices.

Energy minimization on compact spaces

Optimality in Euclidean space has implications for other geometries.

Theorem (Hardin-Saff, 2005)

Let $S \subset \mathbb{R}^3$ be a surface with surface measure 1 and let

$$E_s(S, N) = \inf_{x_1, \ldots, x_N \in S} \sum_{i \neq j} \frac{1}{|x_i - x_j|^{2s}}$$

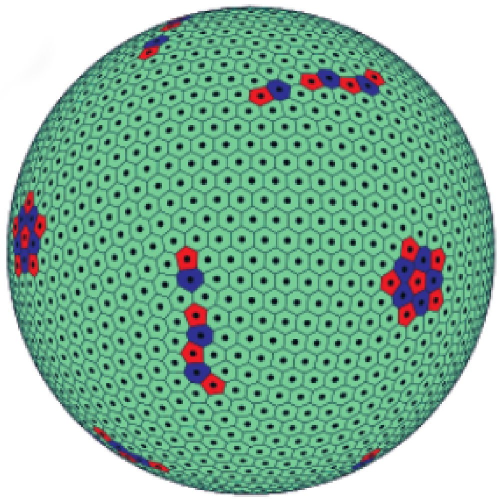
Then for $s > 1$ there exists a universal constant C_s such that

$$E_s(S, N) \sim C_s N^{1+s}, \qquad N \to \infty$$

If A_2 is optimal for s-Riesz energy, then

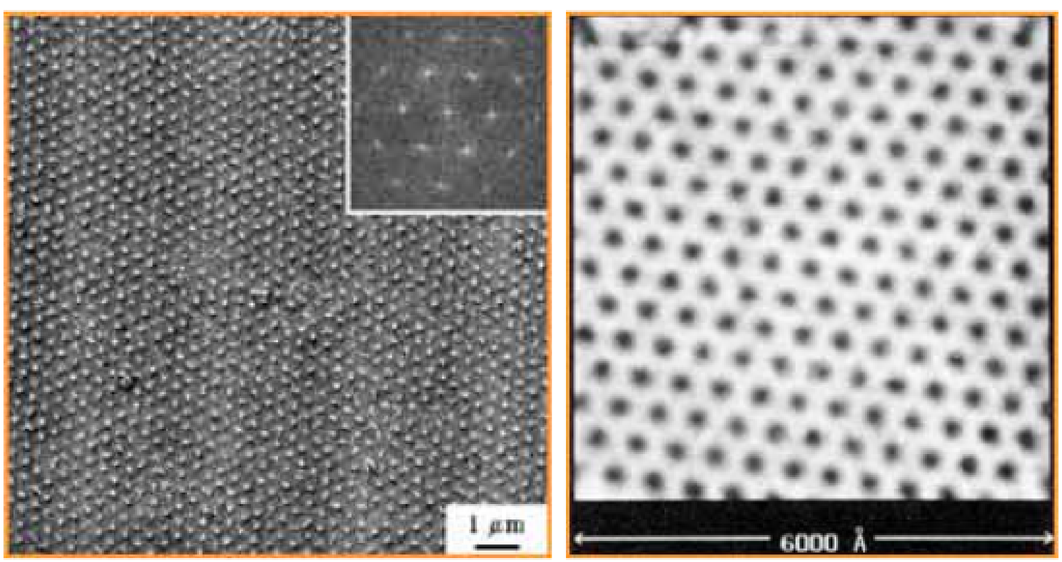
$$C_s = (\sqrt{3}/2)^s \zeta_{\mathbb{Q}(\sqrt{-3})}(s)$$

Energy minimization on the sphere



Hardin, Saff, Notices of the AMS Vol. 51, No 10 (2004)

Superconducting vortices (Abrikosov lattices)



L. Ya. Vinnikov et al. Phys. Rev. B 67, 092512 (2003)

H. F. Hess et al. Phys. Rev. Lett. 62, 214 (1989)

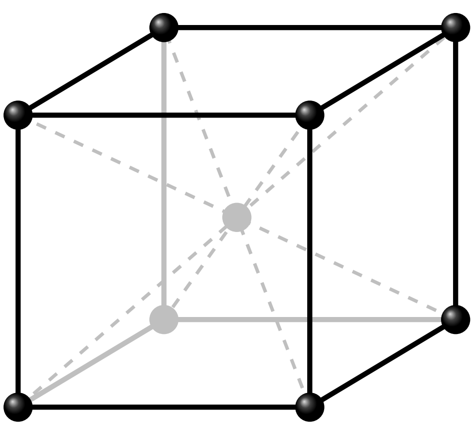
Gaussian core model in $\mathbb{R}^3$

F. Stillinger (1976): for $p(r) = \exp(-\pi r)$ the best configuration varies a lot.

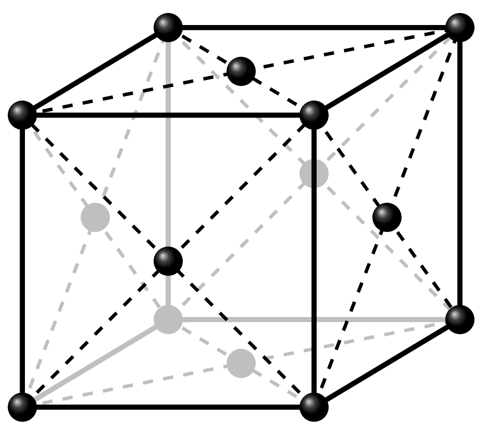
- Density $\rho \ll 1$: fcc-lattice (conjecturally optimal among lattices)
- Density $\rho \gg 1$: bcc-lattice (conjecturally optimal among lattices).
- Density $\rho \approx 1$: some aperiodic configurations are better!
  For $\rho \in (0.99899854..., 1.00100312...)$ one gets 0.0004% improvement.

All of this is conjectural based on numerical experiments.

Conjecturally optimal lattices in $\mathbb{R}^3$



body-centered cubic



face-centered cubic

Universal optimality

Definition

A configuration $\mathcal{C}$ is called universally-optimal, if it minimizes p-energy for all completely monotone functions $p\colon (0,\infty) \to \mathbb{R}$.

- Riesz potentials and Gaussian potentials are completely monotone.
- Gaussian potentials span the cone of completely monotone functions (S. N. Bernstein).

Conjecture (Cohn, Kumar)

In dimensions 1, 2, 8, *and* 24 *the configurations given by* $\mathbb{Z}$, A_2*-lattice*, E_8*-lattice, and the Leech lattice respectively are universally optimal.*

Theorem (Cohn, Kumar)

$\mathbb{Z}$ *is universally optimal.*

Universal optimality of E_8 and Λ_{24}

Theorem (Cohn, Kumar, Miller, R., Viazovska)

The E_8*-lattice and the Leech lattice are universally optimal.*

$$\Lambda_8 = \{(x_1, \dots, x_8) \in \mathbb{Z}^8 \cup (\tfrac{1}{2} + \mathbb{Z})^8 \mid x_1 + \dots + x_8 \equiv 0 \pmod 2\}$$

Construction of the Leech lattice Λ_{24} is much more involved.

Λ_8 and Λ_{24} are even unimodular lattices:

$$\Lambda = \Lambda^* := \{x \in \mathbb{R}^d \mid \langle x, \nu \rangle \in \mathbb{Z} \quad \forall \nu \in \Lambda\},$$

$$\|x\|^2 \in 2\mathbb{Z} \quad \text{for all} \quad x \in \Lambda.$$

Linear programming

Define Fourier transform by $\widehat{f}(\xi) = \int_{\mathbb{R}^d} f(x) e^{-2\pi i \langle x, \xi \rangle} dx$.

Theorem (Cohn-Elkies, Cohn-Kumar)

Let $f : \mathbb{R}^d \to \mathbb{R}$ be a Schwartz function such that

$$\begin{aligned} f(x) &\le p(|x|^2), & x &\ne 0, \\ \widehat{f}(\xi) &\ge 0, & \xi &\in \mathbb{R}^d. \end{aligned}$$

Then any subset $\mathcal{C} \subset \mathbb{R}^d$ of density ρ satisfies

$$E_p(\mathcal{C}) \ge \rho \widehat{f}(0) - f(0)$$

Cohn and Kumar gave a proof when $\mathcal{C}$ is periodic. General case is due to Cohn and de Courcy-Ireland.
For simplicity, assume that $\mathcal{C}$ is periodic, i.e., $\mathcal{C} = \sqcup_{i=1}^{N} (v_i + \Lambda)$, where Λ is a lattice.

Linear programming

Proof.

Poisson summation formula: $\sum_{x \in \Lambda} f(x + v) = \frac{1}{|\Lambda|} \sum_{\xi \in \Lambda^*} \widehat{f}(\xi) e^{2\pi i \xi \cdot v}$

$$\begin{aligned} E_p(\mathcal{C}) &= \frac{1}{N} \sum_{j,k=1}^{N} \sum_{x \in \Lambda \setminus \{v_k - v_j\}} p(|x + v_j - v_k|^2) \\ &\ge \frac{1}{N} \sum_{j,k=1}^{N} \sum_{x \in \Lambda \setminus \{v_k - v_j\}} f(x + v_j - v_k) = \\ &= -f(0) + \frac{1}{N} \sum_{j,k=1}^{N} \sum_{x \in \Lambda} f(x + v_j - v_k) = \\ &= -f(0) + \frac{1}{N|\Lambda|} \sum_{\xi \in \Lambda^*} \widehat{f}(\xi) \Big| \sum_{j=1}^{N} e^{2\pi i \xi \cdot v_j} \Big|^2 \ge \rho \widehat{f}(0) - f(0) \end{aligned}$$

$\square$

Sufficient condition for optimality

Corollary

Let $f\colon \mathbb{R}^d \to \mathbb{R}$ be a Schwartz function such that

$$\begin{aligned} f(x) &\le p(|x|^2), && x \neq 0, \\ \widehat{f}(\xi) &\ge 0, && \xi \in \mathbb{R}^d, \\ f(x) &= p(|x|^2), && x \in \Lambda \setminus \{0\}, \\ \widehat{f}(\xi) &= 0, && \xi \in \Lambda^* \setminus \{0\}. \end{aligned}$$

Then $\mathcal{C} = \Lambda$ has optimal p-energy.

For $\Lambda = \Lambda_8$ and radial f this gives conditions on $f(\sqrt{2n})$, $f'(\sqrt{2n})$, $\widehat{f}(\sqrt{2n})$, $\widehat{f}'(\sqrt{2n})$.
By Bernstein's theorem it is enough to look at $p(r) = e^{-\pi\alpha r}$.

Fourier Interpolation

One of our main results is that any radial function $f\colon \mathbb{R}^d \to \mathbb{R}$ is uniquely determined by the values $f(\sqrt{2n})$, $f'(\sqrt{2n})$, $\widehat{f}(\sqrt{2n})$, $\widehat{f}'(\sqrt{2n})$:

Theorem (CKMRV)

For $d \in \{8, 24\}$ there exist two sequences of radial Schwartz functions $a_n, b_n \in \mathcal{S}(\mathbb{R}^d)$, $n \ge 0$ such that for any radial Schwartz function f we have

$$f(x) = \sum_{n \ge n_0} a_n(x) f(\sqrt{2n}) + \sum_{n \ge n_0} b_n(x) f'(\sqrt{2n}) + \sum_{n \ge n_0} \widehat{a}_n(x) \widehat{f}(\sqrt{2n}) + \sum_{n \ge n_0} \widehat{b}_n(x) \widehat{f}'(\sqrt{2n})$$

Here $n_0 = 1$ for $d = 8$ and $n_0 = 2$ for $d = 24$.

Fourier Interpolation: reformulation

Let $d = 2k$, $k \in \{4, 12\}$, $n_0 = (k+4)/8$. We want to verify

$$f(x) = \sum_{n \geq n_0} a_n(x) f(\sqrt{2n}) + \sum_{n \geq n_0} b_n(x) f'(\sqrt{2n}) + \sum_{n \geq n_0} \widehat{a_n}(x) \widehat{f}(\sqrt{2n}) + \sum_{n \geq n_0} \widehat{b_n}(x) \widehat{f}'(\sqrt{2n})$$

Let $\tau \in \mathfrak{H}$ and set

$$f_\tau(x) = e^{i\pi\tau x^2}$$

Then

$$\widehat{f_\tau}(\xi) = \tau^{-d/2} f_{-1/\tau}(\xi)$$

Fourier Interpolation: reformulation

The above identity becomes

$$e^{i\pi\tau x^2} = F(\tau) + \tau^{-k} G(-1/\tau)$$

where

$$F(\tau) = F(\tau, x) = \sum_{n \geq n_0} a_n(x) e^{2\pi i n\tau} + (2\pi i \tau) \sum_{n \geq n_0} \sqrt{2n} b_n(x) e^{2\pi i n\tau},$$
$$G(\tau) = G(\tau, x) = \sum_{n \geq n_0} \widehat{a_n}(x) e^{2\pi i n\tau} + (2\pi i \tau) \sum_{n \geq n_0} \sqrt{2n} \widehat{b_n}(x) e^{2\pi i n\tau}.$$

Equivalently, F and G have moderate growth and satisfy

$$F(\tau+2) - 2F(\tau+1) + F(\tau) = 0, \quad G(\tau+2) - 2G(\tau+1) + G(\tau) = 0.$$

Fourier Interpolation: reformulation

Thus we need to find $F, G \colon \mathfrak{H} \to \mathbb{C}$ of moderate growth

$$\begin{cases} F(\tau+2) - 2F(\tau+1) + F(\tau) = 0\,, \\ G(\tau+2) - 2G(\tau+1) + G(\tau) = 0\,, \\ F(\tau) + \tau^{-k} G(-1/\tau) = e^{i\pi\tau x^2}\,, \\ F(\tau), G(\tau) = O(\tau e^{2\pi i n_0 \tau})\,, \qquad \tau \to i\infty\,. \end{cases}$$

The notation really suggests that there are modular forms nearby!

Modular integrals

$$\begin{cases} F(\tau+2) - 2F(\tau+1) + F(\tau) = 0\,, \\ G(\tau+2) - 2G(\tau+1) + G(\tau) = 0\,, \\ F(\tau) + \tau^{-k} G(-1/\tau) = \varphi(\tau) := e^{i\pi\tau x^2} \end{cases}$$

To make this more familiar we vectorize these equations. In terms of $\mathcal{F} \colon \mathfrak{H} \to \mathbb{C}^6$

$$\mathcal{F}(\tau) = (F(\tau), F(\tau+1), \tau^{-k}F(1-1/\tau), G(\tau), G(\tau+1), \tau^{-k}G(1-1/\tau))^T$$

the system of equations becomes

$$\begin{cases} \mathcal{F}(\tau) - A_T^{-1}\mathcal{F}(\tau+1) & = \ \psi_T(\tau)\,, \\ \mathcal{F}(\tau) - A_S^{-1}\tau^{-k}\mathcal{F}(-1/\tau) & = \ \psi_S(\tau)\,. \end{cases}$$

Modular integrals

$$A_T = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & 2 & 0 & 0 & 0 & 0 \\ 2 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 & 2 & 0 \\ 0 & 0 & 1 & 2 & 0 & 0 \end{pmatrix}, \qquad A_S = \begin{pmatrix} 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}.$$

$$\psi_T = \begin{pmatrix} 0 \\ 0 \\ 2\varphi|S - \varphi|T^{-1}S \\ 0 \\ 0 \\ 2\varphi - \varphi|TST \end{pmatrix}, \qquad \psi_S = \begin{pmatrix} \varphi \\ 0 \\ 0 \\ \varphi|S \\ 0 \\ 0 \end{pmatrix}.$$

Modular integrals

How to solve such equations? To make life easier let's look at the scalar version.

$$\begin{cases} F(\tau) - F(\tau+1) & = \psi_T(\tau)\,, \\ F(\tau) - \tau^{-k}F(-1/\tau) & = \psi_S(\tau)\,. \end{cases}$$

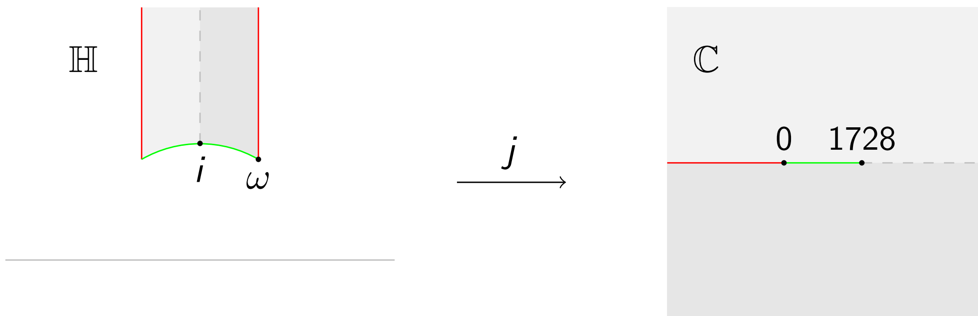
Using modular Green's functions:

$$F(\tau) = \int_i^{\omega} K(\tau,z)\psi_S(z)dz + \int_{\omega}^{i\infty} K(\tau,z)\psi_T(z)dz\,, \qquad \tau \in \mathcal{D}$$

- $K(\tau,z)$ is modular of weight k in τ
- $K(\tau,z)$ is modular of weight $2-k$ in z
- $K(\tau,z)$ has simple poles only at $z \in \mathrm{PSL}_2(\mathbb{Z})\tau$ with residue $1/(2\pi i)$ at $z=\tau$
- "good behavior at the cusps"

Modular integrals as a boundary value problem

For $k = 0$ we have $K(\tau, z) = \frac{1}{2\pi i} \frac{j'(z)}{j(z) - j(\tau)} = \frac{E_{14}(z)/\Delta(z)}{j(\tau) - j(z)}$



- Enough to satisfy the equations for F on the closure of the fundamental domain.
- Change of variable $w = j(\tau)$ gives $\widetilde{F}\colon \mathbb{C} \setminus (-\infty, 1728] \to \mathbb{C}$ with prescribed jumps along $(-\infty, 0)$ and $(0, 1728)$.
- After the change of variables $K(\tau, z)$ becomes the Cauchy kernel.

Issues in the vector-valued case

To construct $K(\tau, z)$ explicitly in the vector-valued case there are some obstacles.

- $\psi_T(\tau)$ and $\psi_S(\tau)$ need to satisfy the cocycle relations. (Luckily they do.)
- The representation of $\mathrm{PSL}_2(\mathbb{Z})$ needs to be of “polynomial growth”.
- Explicit description of vector-valued modular forms (VVMF): the 6D representation splits into two 3D. VVMF for one of them are essentially quasimodular forms of depth 2; the other involves $\log(\lambda(\tau))$, $\log(1 - \lambda(\tau))$.

Modular integrals

Going back to the original problem.

- From matrix-valued modular Green's functions we obtain

$$F(\tau, x) = e^{i\pi\tau x^2} + \sin^2(\pi x^2/2) \int_0^\infty K(\tau, it) e^{-\pi t x^2} dt$$

  where $K(\tau, z)$ is an explicit kernel.
- Universal optimality follows from $K(i\alpha, it) \geq 0$ for all $\alpha, t > 0$.
- This inequality is verified with a help of a computer.

Open problem

Conjecture

Let $d, l > 0$. If $f \in \mathcal{S}_{rad}(\mathbb{R}^d)$ satisfies $f^{(j)}(\sqrt{ln}) = \widehat{f}^{(j)}(\sqrt{ln})$ for all $n \geq 0$ and $0 \leq j < l$, then $f = 0$.

For $l = 1, 2$ this can be proved using the same techniques as in our proof.
For $l \geq 3$ the method does not work. For $l = 3$ it reduces to understanding solutions to

$$\begin{cases} F(\tau+2) - 3F(\tau+4/3) + 3F(\tau+2/3) - F(\tau) & = 0\,, \\ F(\tau) \pm \tau^{-k} F(-1/\tau) & = 0\,. \end{cases}$$

Are there any solutions?
Are the solution spaces finite-dimensional?