Title: Sphere packings, universal optimality, and Fourier interpolation

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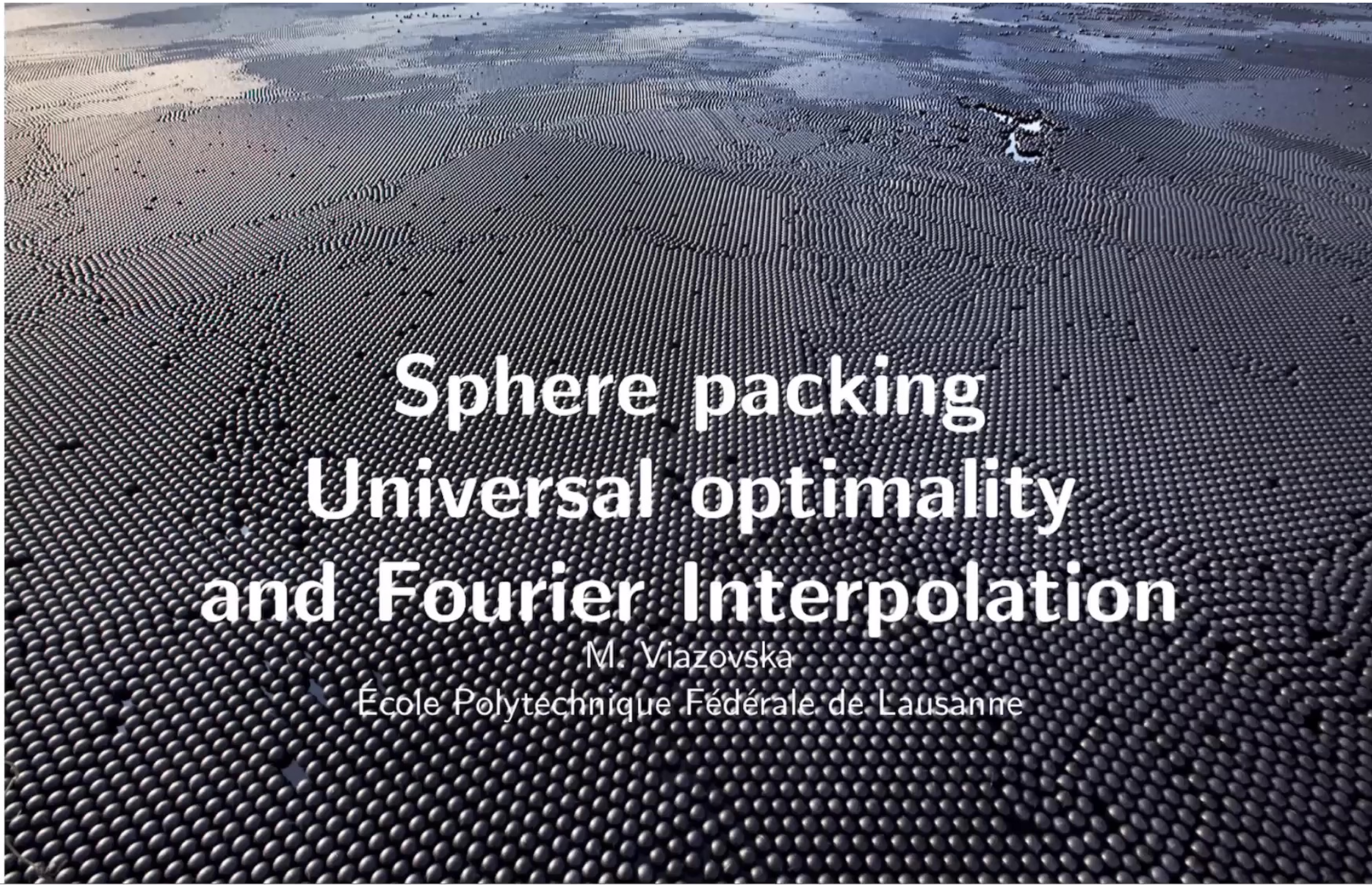
Abstract: In this lecture we will show that the E8 and Leech lattices minimize energy of every potential function that is a completely monotonic function of squared distance (for example, inverse power laws or Gaussians). This theorem implies recently proven optimality of E8 and Leech lattices as sphere packings and broadly generalizes it to long-range interactions. The key ingredient of the proof is sharp linear programming bounds. To construct the optimal auxiliary functions attaining these bounds, we prove a new interpolation theorem. This is the joint work with Henry Cohn, Abhinav Kumar, Stephen D. Miller, and Danylo Radchenko.



Sphere packing Universal optimality and Fourier Interpolation

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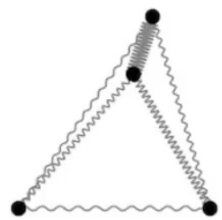
Potential energy

Let $\mathcal{C}$ be a finite subset $\mathbb{R}^d$. Fix a *potential function* $p\colon (0,\infty) \to \mathbb{R}$.



The *potential* p*-energy* of $\mathcal{C}$ is

$$\frac{1}{|\mathcal{C}|} \sum_{\substack{x,y\in\mathcal{C}\\ x\neq y}} p\big(|x-y|\big).$$

Potential energy

Let $\mathcal{C}$ be a discrete, closed subset of $\mathbb{R}^d$. We say $\mathcal{C}$ has *density* ρ if

$$\lim_{r\to\infty} \frac{\left|\mathcal{C} \cap B_d(0,r)\right|}{\mathrm{vol}\big(B_d(0,r)\big)} = \rho.$$

The *lower p-energy* of $\mathcal{C}$ is

$$E_p(\mathcal{C}) := \liminf_{r\to\infty} \frac{1}{\left|\mathcal{C} \cap B_d(0,r)\right|} \sum_{\substack{x,y\in\mathcal{C}\cap B_d(0,r)\\ x\neq y}} p\big(|x-y|\big).$$

The limit exists $\implies$ we call $E_p(\mathcal{C})$ the *p-energy* of $\mathcal{C}$.
For some important p this limit does not exist (e. g. Coulomb energy).

Example 1

Lattices

Let $\Lambda \subset \mathbb{R}^d$ be a *lattice*, i. e. a discrete abelian subgroup of rank d.
The density of Λ is

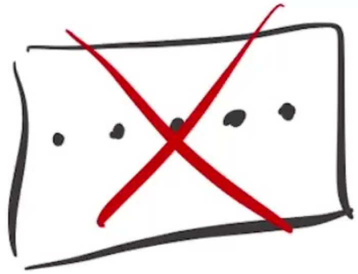
$$\rho(\Lambda) = \frac{1}{\mathrm{vol}(\mathbb{R}^d/\Lambda)}.$$

The p-energy of Λ is

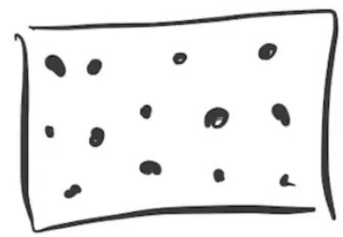
$$E_p(\Lambda) = \sum_{x \in \Lambda \setminus \{0\}} p(|x|).$$

Example 1

$(0,h)$



$\mathbb{R}^2$



$\mathbb{R}^2$ $\mathbb{Z}^2$

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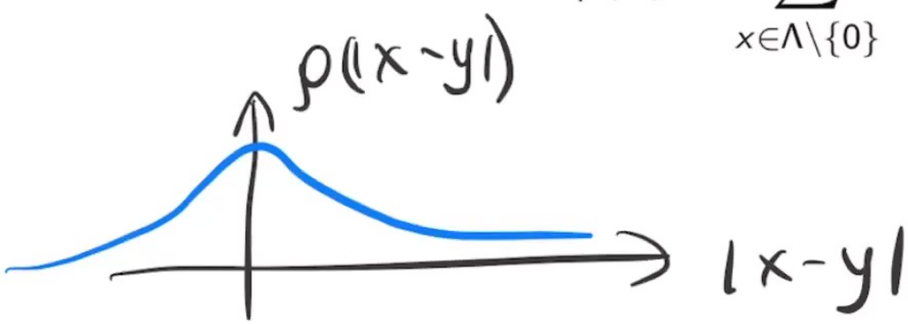


Example 2

Periodic configurations

Fix a lattice $\Lambda \subset \mathbb{R}^d$. A configuration $\mathcal{C} \subset \mathbb{R}^d$ is Λ-*periodic* if $\mathcal{C} + \ell = \mathcal{C}$ for all $\ell \in \Lambda$.
The density of C is

$$\frac{|\mathcal{C}/\Lambda|}{\mathrm{vol}(\mathbb{R}^d/\Lambda)}.$$

The p-energy of $\mathcal{C}$ is

$$E_p(\mathcal{C}) = \frac{1}{|\mathcal{C}/\Lambda|}\Big(\sum_{\substack{x,y \in \mathcal{C}/\Lambda \\ x \neq y}} \sum_{\ell \in \Lambda} p(x - y + \ell)\Big) + \sum_{\ell \in \Lambda \setminus \{0\}} p(\ell)$$

$$= \frac{1}{|\mathcal{C}/\Lambda|}\Big(\sum_{x,y \in \mathcal{C}/\Lambda} \sum_{\ell \in \Lambda} p(|x - y + \ell|)\Big) - p(0).$$

Potential energy minimization

Let $\mathcal{C}$ be a discrete subset of $\mathbb{R}^d$ with density ρ, where $\rho > 0$, and let $p\colon (0,\infty) \to \mathbb{R}$ be any function.

We say that $\mathcal{C}$ *minimizes energy for p* if its p-energy $E_p(\mathcal{C})$ exists and every configuration in $\mathbb{R}^d$ of density ρ has lower p-energy at least $E_p(\mathcal{C})$.

We also call $\mathcal{C}$ a *ground state* for p.

Universal optimality

How do the ground states depend on the energy profile p?

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

Fix $\alpha > 0$ and set

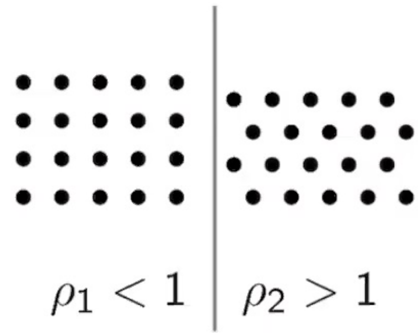
$$p_\alpha(r) = e^{-\pi\alpha r^2}.$$

Consider configurations of density $\rho = 1$.

$\alpha \ll 1$ bcc lattice

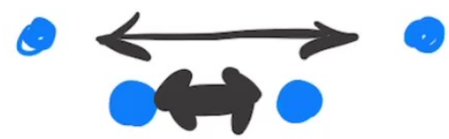
$\alpha \gg 1$ fcc lattice

$\alpha \approx 1$ F. Stillinger (1976): Phase coexistence has smaller energy then fcc and bcc.



$\rho_1 < 1$ | $\rho_2 > 1$

Universal optimality



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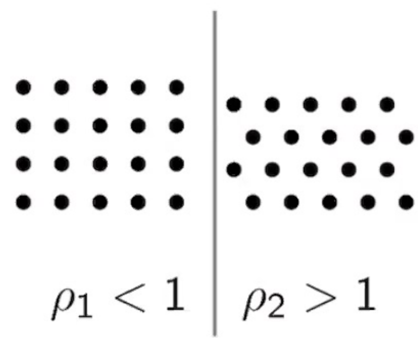

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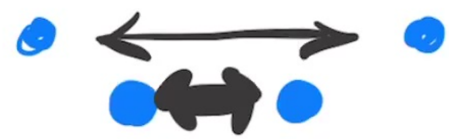

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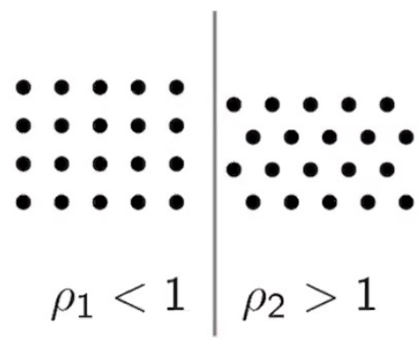
Poisson summation

$$E_{p_1}(bcc) = E_{p_1}(fcc)$$



Universal optimality

Let $\mathcal{C}$ be a discrete subset of $\mathbb{R}^d$ with density ρ, where $\rho > 0$. We say $\mathcal{C}$ is *universally optimal* if it minimizes p-energy whenever $p\colon (0,\infty) \to \mathbb{R}$ is a completely monotonic function of squared distance. (equivalent to minimazing p_α - energy for all $\alpha \in \mathbb{R}_{>0}$)

Conjecture(Cohn, Kumar)

The lattices $\mathbb{Z}, A_2, \Lambda_8$ and Λ_{24} are universally optimal.

Theorem (Cohn, Kumar 2007)

The lattice $\mathbb{Z}$ is universally optimal.

Theorem (Cohn, Kumar, Miller, Radchenko, V 2019)

The lattices Λ_8 and Λ_{24} are universally optimal.

Our strategy of the proof

- Linear programming bounds
- Fourier interpolation
- Numerical verification of the positivity of a certain function on $[0, 1] \times [0, 1]$.

Linear programming bounds

Theorem(Cohn, Kumar)

Let $p\colon (0,\infty) \to \mathbb{R}$ be any function, and suppose $f : \mathbb{R}^d \to \mathbb{R}$ is a Schwartz function. If $f(x) \leq p\big(|x|\big)$ for all $x \in \mathbb{R}^d \setminus \{0\}$ and $\widehat{f}(y) \geq 0$ for all $y \in \mathbb{R}^d$, then every subset of $\mathbb{R}^d$ with density ρ has lower p-energy at least $\rho\widehat{f}(0) - f(0)$.

Linear programming bounds

f is a Schwartz function

$f \in C^\infty(\mathbb{R}^d)$ $\qquad |x|^\alpha \mathcal{D}_\beta(f)(x) \to 0$ as $|x| \to \infty$

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Fourier transform

$$\widehat{f}(y) = \int_{\mathbb{R}^d} f(x)\, e^{-2\pi i x y}\, dx$$

Cohn-Kumar linear programming bound. Idea of the proof

Let $\mathcal{C} \subset \mathbb{R}^d$ be a Λ-periodic configuration of density ρ.

$$E_p(\mathcal{C}) = \frac{1}{|\mathcal{C}/\Lambda|}\Big(\sum_{\substack{x,y\in\mathcal{C}/\Lambda \\ x\neq y}} \sum_{\ell\in\Lambda} p(x-y+\ell)\Big) + \sum_{\ell\in\Lambda\setminus\{0\}} p(\ell)$$

$$\geq \frac{1}{|\mathcal{C}/\Lambda|}\Big(\sum_{\substack{x,y\in\mathcal{C}/\Lambda \\ x\neq y}} \sum_{\ell\in\Lambda} f(x-y+\ell)\Big) + \sum_{\ell\in\Lambda\setminus\{0\}} f(\ell) = \frac{1}{|\mathcal{C}/\Lambda|}\Big(\sum_{x,y\in\mathcal{C}/\Lambda} \sum_{\ell\in\Lambda} f(x-y+\ell)\Big) - f(0)$$

Use the Poisson summation f-la

$$= \frac{1}{|\mathcal{C}/\Lambda|} \sum_{x,y\in\mathcal{C}/\Lambda} \frac{1}{\mathrm{vol}(\mathbb{R}^d/\Lambda)} \left(\sum_{\mu\in\Lambda^*} \widehat{f}(\mu) e^{2\pi i (x-y)\mu} \right) - f(0)$$

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$$= \frac{1}{|\mathcal{C}/\Lambda|} \sum_{x,y \in \mathcal{C}/\Lambda} \frac{1}{\mathrm{vol}(\mathbb{R}^d/\Lambda)} \left(\sum_{\mu \in \Lambda^*} \widehat{f}(\mu) e^{2\pi i (x-y)\mu} \right) - f(0)$$

$$= \frac{1}{|\mathcal{C}/\Lambda| \, \mathrm{vol}(\mathbb{R}^d/\Lambda)} \left(\sum_{\mu \in \Lambda^*} \widehat{f}(\mu) \Big| \sum_{x \in \mathcal{C}/\Lambda} e^{2\pi i x \mu} \Big|^2 \right) - f(0)$$

use

$\widehat{f}(y) \geq 0$

$$\geq \frac{1}{|\mathcal{C}/\Lambda| \, \mathrm{vol}(\mathbb{R}^d/\Lambda)} |\widehat{f}(0)| \cdot |C/\Lambda|^2 - f(0) = \rho \widehat{f}(0) - f(0).$$

Sharp linear programming bounds

Suppose that a lattice $\Lambda \subset \mathbb{R}^d$ minimizes p-energy for some $p : (0, \infty) \to \mathbb{R}$.

Suppose that the optimality can be proven by linear programming using a Schwartz function $f : \mathbb{R}^d \to \mathbb{R}$.

No loss in the inequalities $\Longrightarrow$

- $f(x) = p(|x|)$ for all $x \in \Lambda \setminus \{0\}$
- $\widehat{f}(y) = 0$ for all $y \in \Lambda^* \setminus \{0\}$
- Equalities hold to the second order

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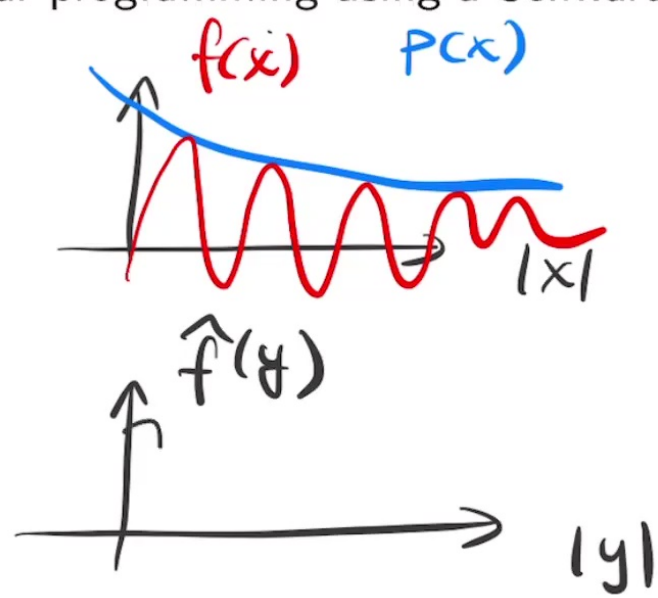

Fourier interpolation of second order

Theorem (2019)

Let (d, n_0) be $(8, 1)$ or $(24, 2)$. There exists a collection of radial Schwartz functions $a_n, b_n, \widetilde{a}_n, \widetilde{b}_n : \mathbb{R}^d \to \mathbb{R}$ such that for every $f \in \mathcal{S}_{\text{rad}}(\mathbb{R}^d)$ and $x \in \mathbb{R}^d$,

$$f(x) = \sum_{n=n_0}^{\infty} f\left(\sqrt{2n}\right) a_n(x) + \sum_{n=n_0}^{\infty} f'\left(\sqrt{2n}\right) b_n(x) + \sum_{n=n_0}^{\infty} \widehat{f}\left(\sqrt{2n}\right) \widetilde{a}_n(x) + \sum_{n=n_0}^{\infty} \widehat{f}'\left(\sqrt{2n}\right) \widetilde{b}_n(x),$$

and these series converge absolutely.

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and these series converge absolutely.

$\{\sqrt{2n}\}_{n \in \mathbb{Z}_{\geq n_0}} \leftarrow$ lengths of non-zero vectors Λ_d

Fourier interpolation

- D. Radchenko, M. V. - Fourier interpolation on the real line (2017)
- A. Bondarenko, D. Radchenko, K. Seip - Fourier interpolation with zeros of zeta and L-functions (2020)
- J. Ramos, M. Sousa, Perturbed interpolation formulae and applications
- M. Sodin, A. Kulikov, F. Nazarov - Fourier uniqueness and non-uniqueness pairs (2020)

Construction of "Magic functions"

Let $p : (0, \infty) \to \mathbb{R}$ be a completely monotonic potential function. The only possible "magic" function f that could prove a sharp bound for E_8 or the Leech lattice under a potential p:

$$f(x) = \sum_{n=n_0}^{\infty} p\big(\sqrt{2n}\big)\, a_n(x) + \sum_{n=n_0}^{\infty} p'\big(\sqrt{2n}\big)\, b_n(x).$$

In order to prove that E_8 or the Leech lattice minimize the p-energy, it suffices to show that $f(x) \leq p\big(|x|\big)$ for all $x \in \mathbb{R}^d \setminus \{0\}$ and $\widehat{f}(y) \geq 0$ for all $y \in \mathbb{R}^d$.

If a configuration is a ground state for every Gaussian $r \mapsto e^{-\alpha r^2}$, then the same is true for every completely monotonic function of squared distance.

Functional equation for the "magic function"

Consider the generating functions

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

and

$$\widetilde{F}(\tau, x) = \sum_{n \geq n_0} \widetilde{a}_n(x)\, e^{2\pi i n \tau} + 2\pi i \tau \sum_{n \geq n_0} \sqrt{2n}\, \widetilde{b}_n(x)\, e^{2\pi i n \tau},$$

The interpolation formula for the complex Gaussian $x \mapsto e^{\pi i \tau |x|^2}$ is equivalent to

$$F(\tau, x) + (i/\tau)^{d/2} \widetilde{F}(-1/\tau, x) = e^{\pi i \tau |x|^2}.$$

Functional equation for the "magic function"

$\tau \in \mathbb{C}, \ \mathrm{Im}(\tau) > 0$

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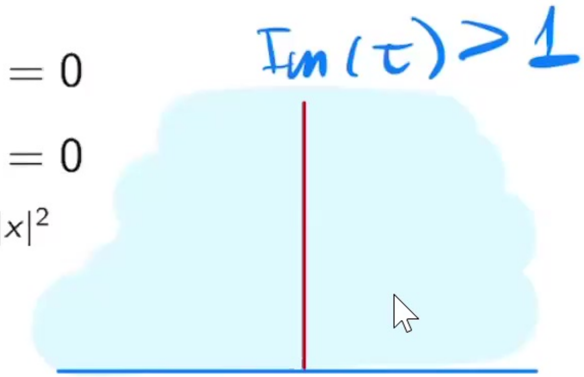
Solving the functional equation

Using the methods developed in the theory of automorphic forms and by improving these techniques we can *explicitly* solve the functional equation

$$F(\tau+2,x)-2F(\tau+1,x)+F(\tau,x)=0$$
$$\widetilde{F}(\tau+2,x)-2\widetilde{F}(\tau+1,x)+\widetilde{F}(\tau,x)=0$$
$$F(\tau,x)+(i/\tau)^{d/2}\widetilde{F}(-1/\tau,x)=e^{\pi i\tau|x|^2}$$



Moderate growth of F implies the interpolation formula

The inequality $\widetilde{F}(it,x)>0$ for $t\in(0,\infty)$ implies the universal optimality of Λ_8 and Λ_{24}.

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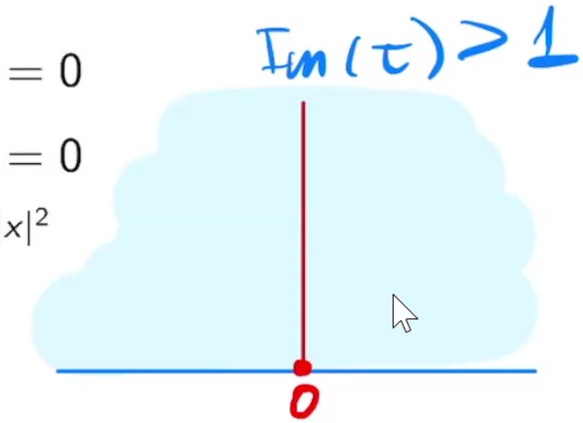

Moderate growth of F implies the interpolation formula

$f \le P \qquad \hat{f} \geq 0$

The inequality $\widetilde{F}(it,x) > 0$ for $t \in (0,\infty)$ implies the universal optimality of Λ_8 and Λ_{24}.

Technical details of the proof.