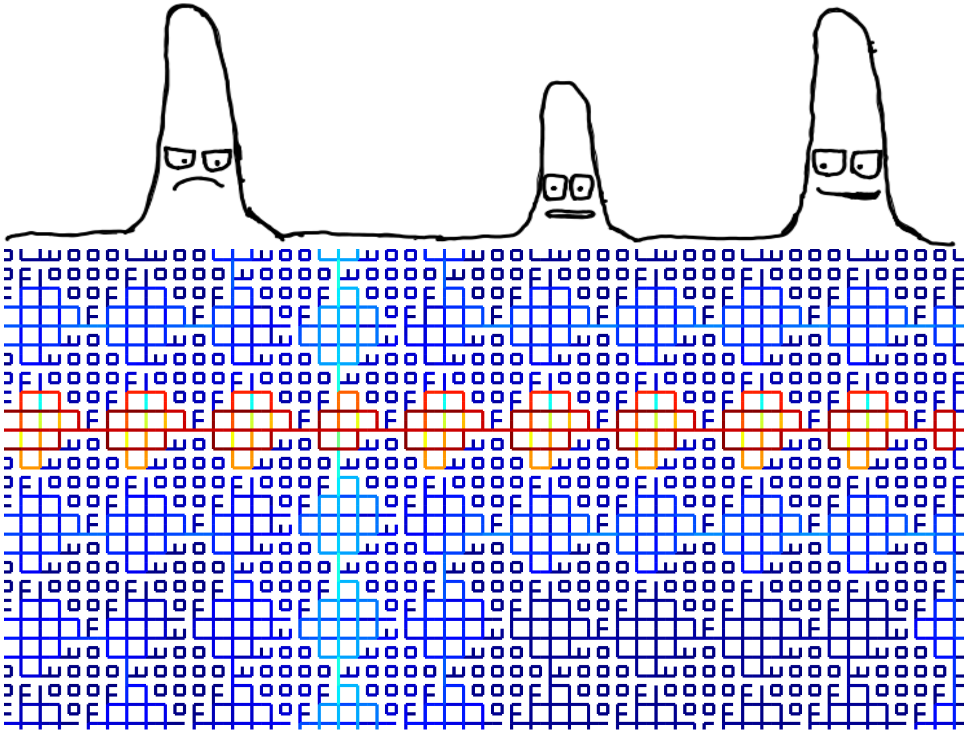
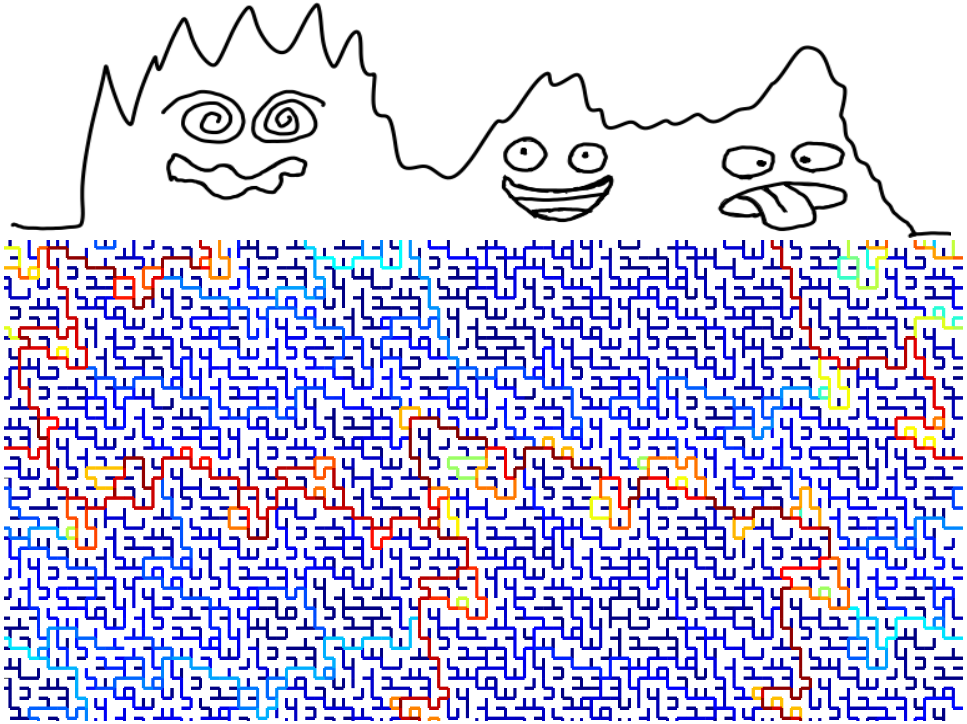
Order to Disorder in Quasiperiodic Systems





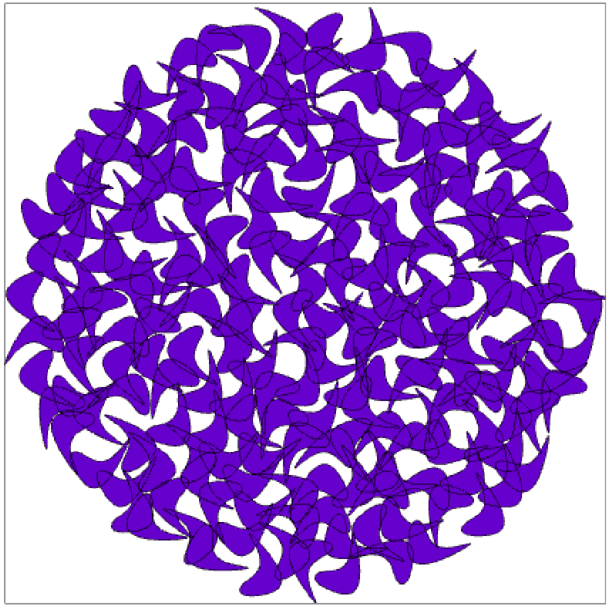
David Morison*, N. Benjamin Murphy**,
Elena Cherkaev**, Kenneth M. Golden**

* Department of Physics & Astronomy, University of Utah
** Department of Mathematics, University of Utah

Presented at 2020 Annual Meeting of the APS Four Corners Section

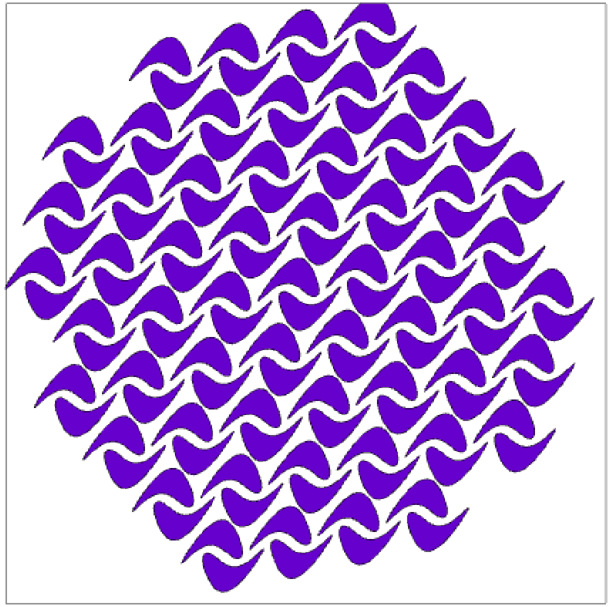
Materials Science Before the 80's

Disordered



Amorphous, Glass Like

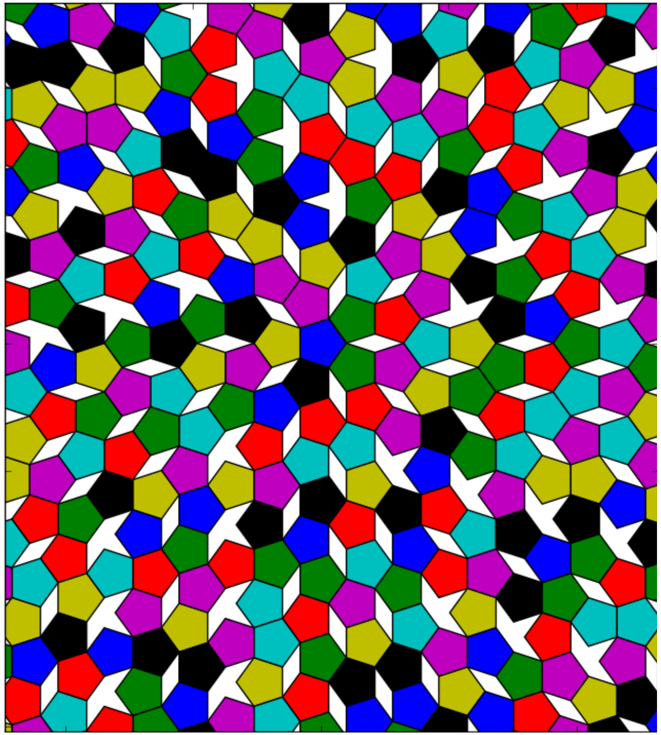
Periodic



Crystalline, Translational Symmetry

Quasiperiodic Tilings are for Art and Math, Not for Materials Science?

Green Mosque in Bursa, Turkey



2D tiling with pentagons and gaps

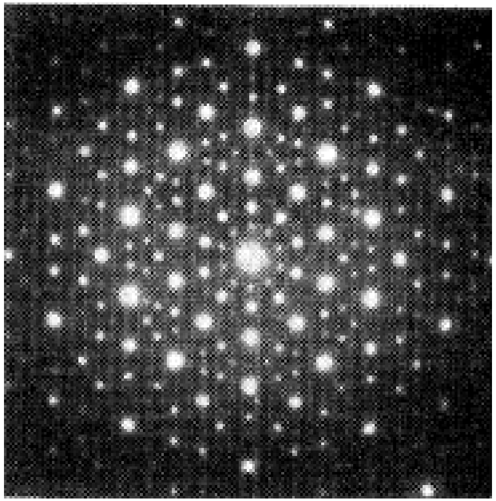
Roger Penrose

Experimental Discovery

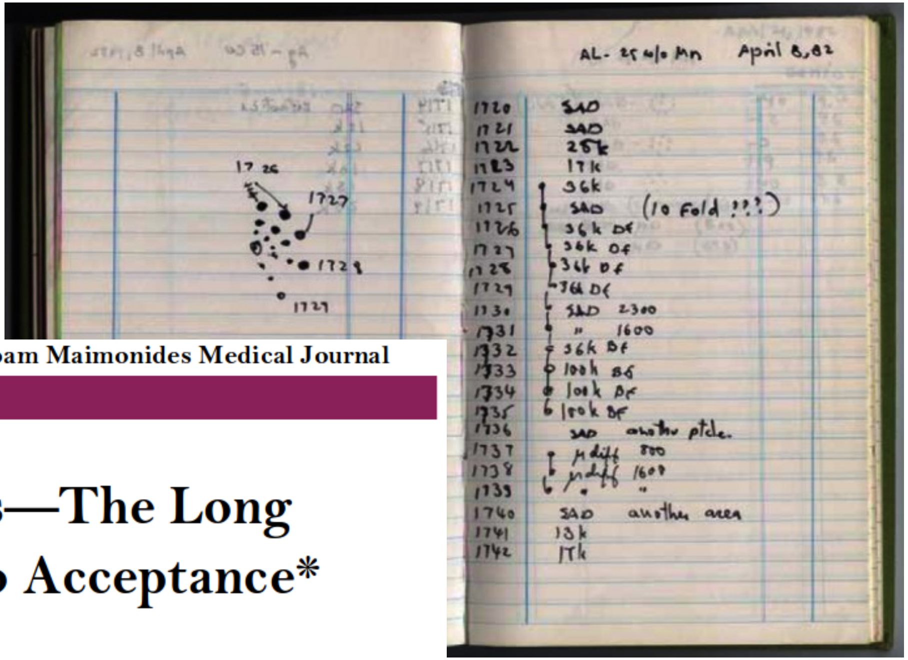
VOLUME 53, NUMBER 20 PHYSICAL REVIEW LETTERS 12 NOVEMBER 1984

Metallic Phase with Long-Range Orientational Order and No Translational Symmetry

D. Shechtman and I. Blech
Department of Materials Engineering, Israel Institute of Technology–Technion, 3200 Haifa, Israel



TEM Diffraction pattern
For an AlMg alloy
Notice ten fold symmetry



Open Access Rambam Maimonides Medical Journal

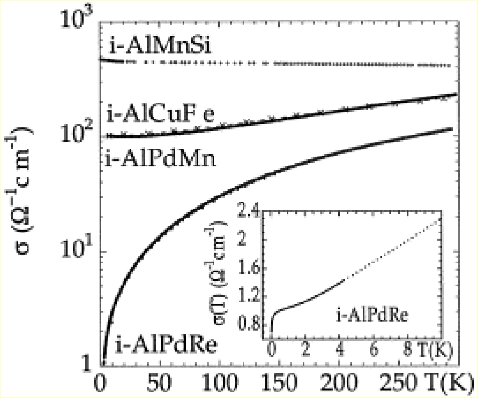
NOBEL LAUREATE PERSPECTIVE

Quasi-Periodic Crystals—The Long Road from Discovery to Acceptance*

Daniel Shechtman, Ph.D.**
Nobel Prize Laureate in Chemistry, 2011. Philip Tobias Professor of Materials Science, Department of Materials Science and Engineering, Technion–Israel Institute of Technology, Haifa, Israel

Discovery of Novel Properties in Molecular Quasicrystals

- Low Electrical Conductivity
- Low Thermal Conductivity
- Mechanically Hard
- Small Coefficient of Friction

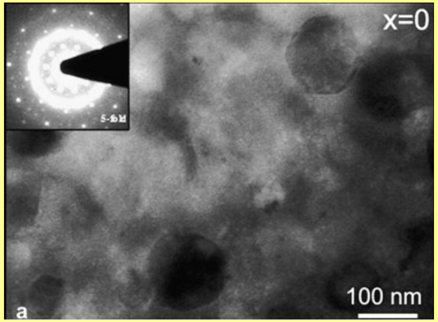


an insulating aluminum alloy

C Berger, C. *et al*. Physica B: Condensed Matter (2000)

water beading more strongly on a quasicrystal coating, than on Teflon

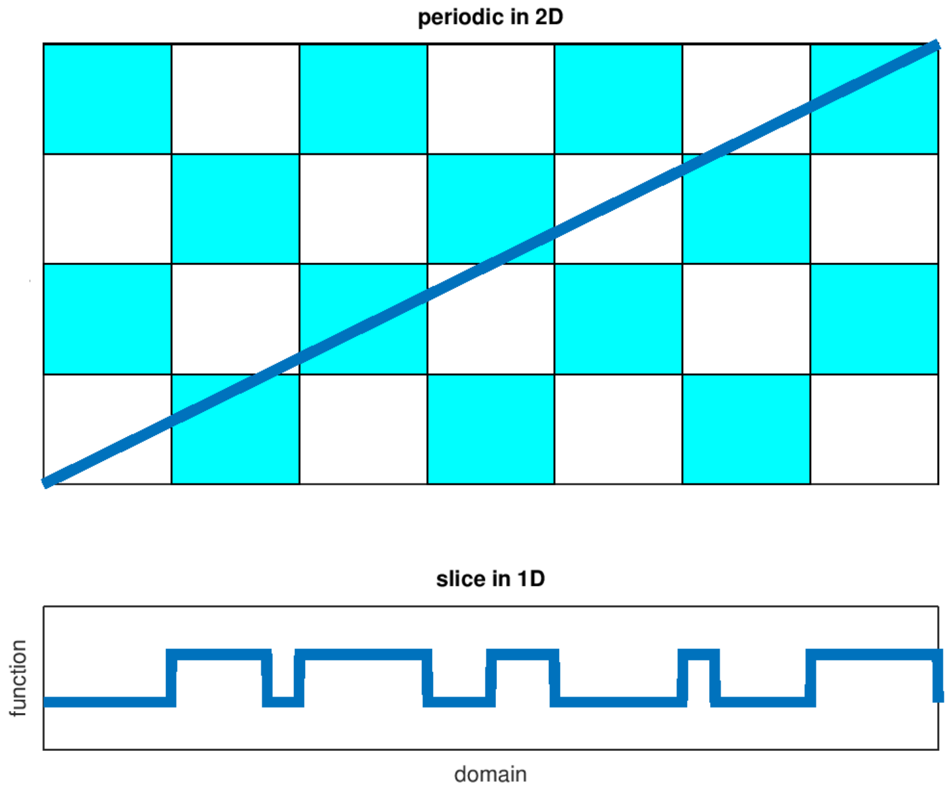
Made by Professor Orest Symko



hard alloy quasicrystal inclusions

Singh. *et al*. Intermetallics (2010)

Interesting Transport in Idealized Quasiperiodic systems



Golden, K. *et al.*
Journal of Statistical Physics
(1990)

1-D

$$\frac{1}{\sigma^*} = \frac{p_1}{\sigma_1} + \frac{1-p_1}{\sigma_2}$$

$$p_1 = \frac{1}{2}\left(1 - \frac{1}{pq}\right)$$

n-D

Golden, K. *et al.* Classical Transport in Modulated Structures
Phys. Rev. Lett. (1985)

Is there an inherent connection between quasiperiodic geometry and material properties?

In a Stieltjes integral, the relationship between microgeometry and bulk properties is distilled into a spectral representation.

Classical not Quantum

We assume that our system is adequately described classically without recourse to the Schrödinger equation.

$$\cancel{i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi}$$

yes ≥ nanometers or 10^3 atoms ≥ no

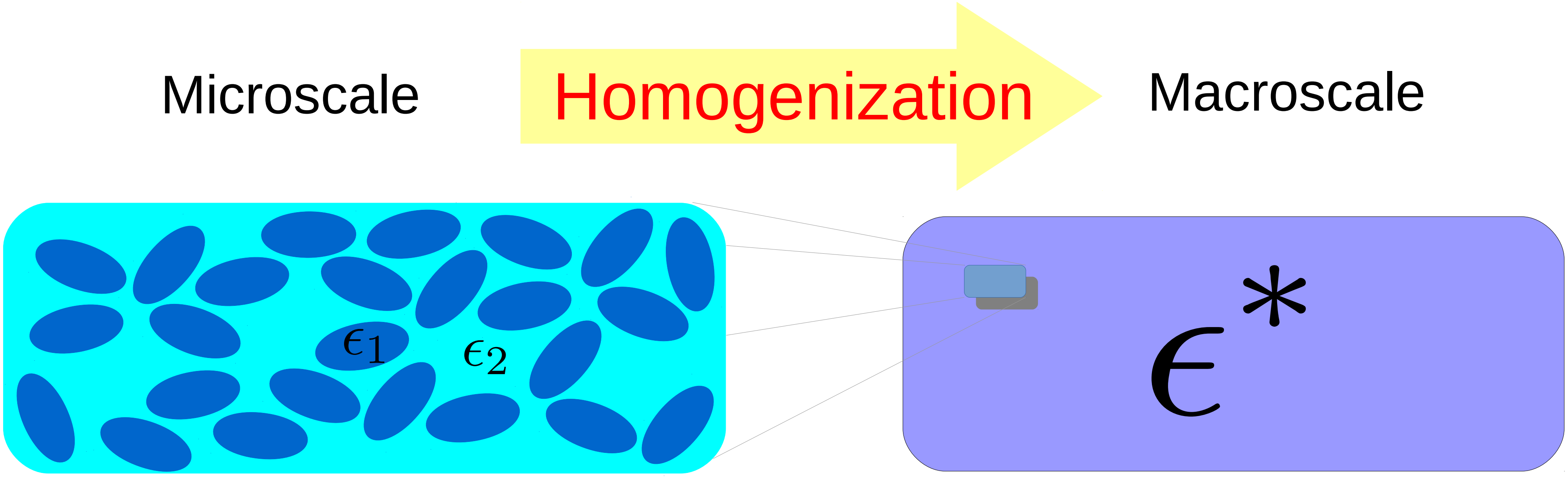
Permittivity

$$\vec{D} = \epsilon\vec{E} = \epsilon_0\vec{E} + \vec{P}$$

Effective Complex Permittivity of a Two Phase Composite in the Quasistatic (Long Wavelength) Limit

$$\epsilon\left(x\right) = \epsilon_1 \chi\left(x\right) + \epsilon_2 \left(1 - \chi\left(x\right)\right)$$

What is the effective permittivity of a material
with periodic, quasiperiodic or random microgeometry?



Relating Composite Geometry to Homogenized Properties

1873 Maxwell: effective conductivity of a dilute suspension of spheres
1906 Einstein: effective viscosity of a dilute suspension of rigid spheres in a fluid

D. Bergman, Physics Reports, 1978
D. Bergman, Phys. Rev. Lett. 1980

G. Milton, Appl. Phys. Lett. 1980
G. Milton, J. Appl. Phys. 1981

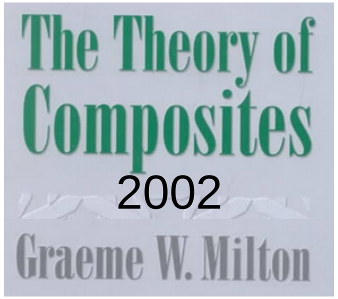
Bounds for Effective Parameters of Heterogeneous Media by Analytic Continuation

Communications in Mathematical Physics

1983

K. Golden* and G. Papanicolaou**

Courant Institute, New York University, New York, NY 10012, USA



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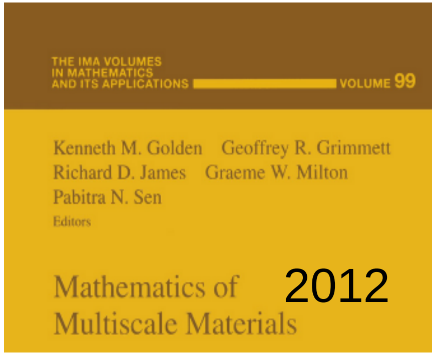
SPECTRAL MEASURE COMPUTATIONS FOR COMPOSITE MATERIALS*

N. BENJAMIN MURPHY†, ELENA CHERKAEV‡, CHRISTEL HOHENEGGER§, AND KENNETH M. GOLDEN¶

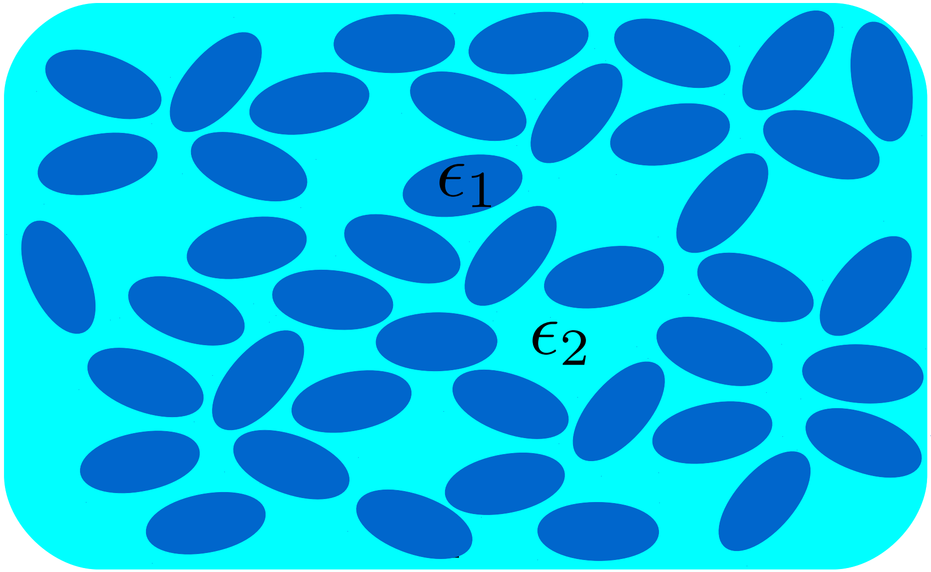
Comm. Math. Sci.

Dedicated to George Papanicolaou on the occasion of his 70th birthday.

2015



Effective Complex Permittivity of a Two Phase Composite in the Quasistatic (Long Wavelength) Limit



$$\left.\begin{array}{c}\vec{D} = \epsilon \vec{E} \\ \nabla \cdot \vec{D} = 0 \\ \nabla \times \vec{E} \approx 0\end{array}\right\} \boldsymbol{\epsilon}^*$$

$$\left\langle \vec{D} \right\rangle = \boldsymbol{\epsilon}^* \left\langle \vec{E} \right\rangle = \boldsymbol{\epsilon}^* \vec{E}_0$$

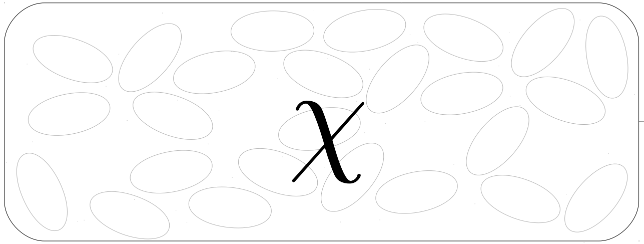
$$\epsilon^* = \epsilon^* \left(\frac{\epsilon_1}{\epsilon_2}, \text{composite geometry} \right)$$

Effective permitivity is a tensor but we simply discuss the isotropic case.

$$\boldsymbol{\epsilon}^* = \epsilon^* \mathrm{I}$$

Stieltjes Integral Representation

Microgeometry



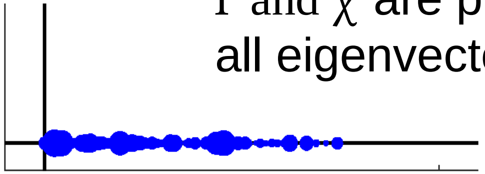
χ

$$\chi\Gamma\chi v_k = \lambda_k v_k$$

Relevant Physics and Boundary Conditions

Γ

$$\mu \text{ or } \lambda_k, \langle \hat{e}, v_k v_k^t \hat{e} \rangle$$



Γ and χ are projection operators
all eigenvectors real and [0,1]

$$1 - \frac{\epsilon^*}{\epsilon_2} = \int_0^1 \frac{d\mu(\lambda)}{s - \lambda}$$

Material Properties

$$s = \frac{1}{1 - \epsilon_1/\epsilon_2}$$

Eigenvalues of $\chi\Gamma\chi$ Correspond to Resonances of the Composite Geometry

In the discrete case the Stieltjes integral becomes a summation.

$$1 - \frac{\epsilon^*}{\epsilon_2} = \sum_k \frac{\langle \hat{e}, v_k v_k^t \hat{e} \rangle}{s - \lambda_k}$$

resonance

$$s = \frac{1}{1 - \epsilon_1/\epsilon_2} \rightarrow \lambda_k$$

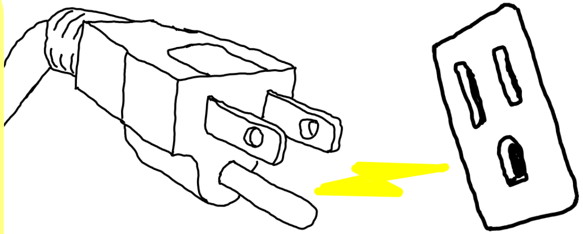
Connected Conductor

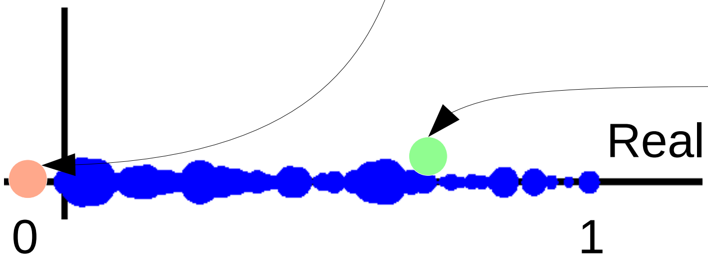
ideal conductor $\sigma_1 \rightarrow \infty$

ideal insulator $\sigma_2 \approx 0$

resonance

$$s \rightarrow \frac{1}{1-\infty}$$





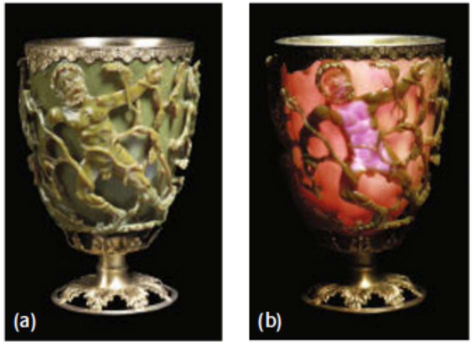
Surface Plasmon Resonance

good metal $\epsilon_1 \approx$ negative real axis

vacuum $\epsilon_2 \approx \epsilon_0$

resonance

$$s \rightarrow (0, 1)$$

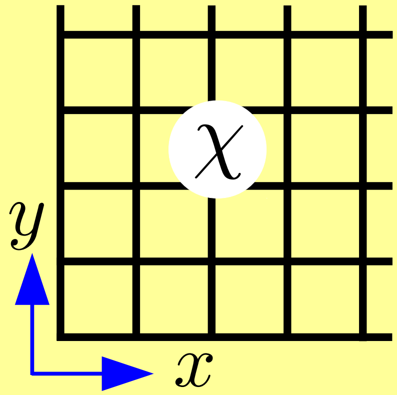


Quasiperiodic in this Context of Materials Science

"...any solid having an essentially discrete diffraction diagram."
International Union of Crystallography

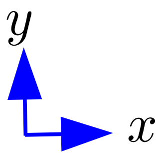
The term "quasicrystal" should simply be regarded as an abbreviation for "quasiperiodic crystal,"
Ron Lifshitz arXiv 2000

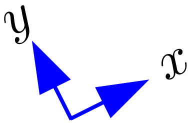
Trial Microgeometry

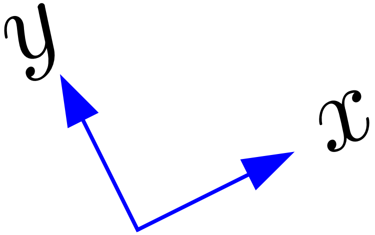


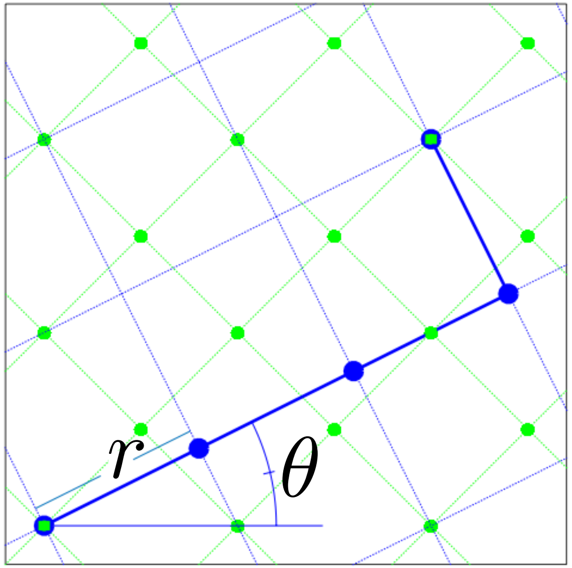
- Deterministic
- Non-periodic
- Repeated Building Blocks

Moiré Pattern Based Trial Geometry







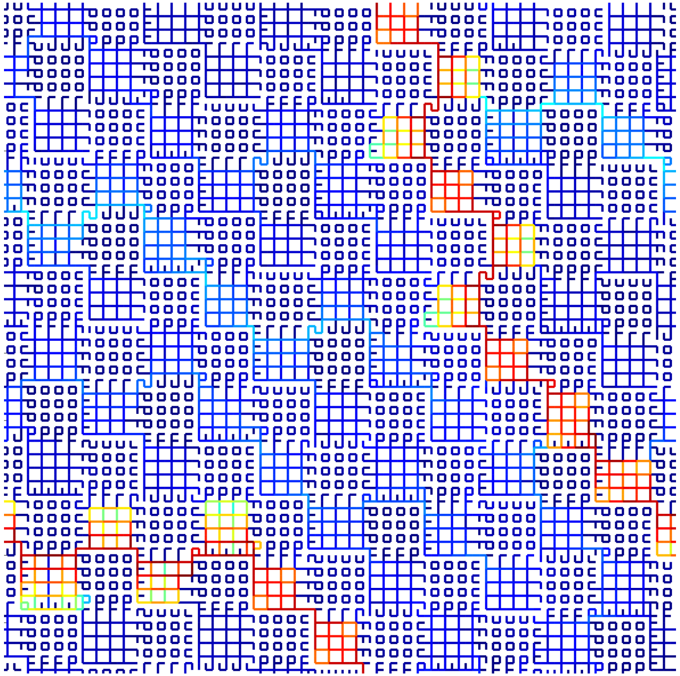


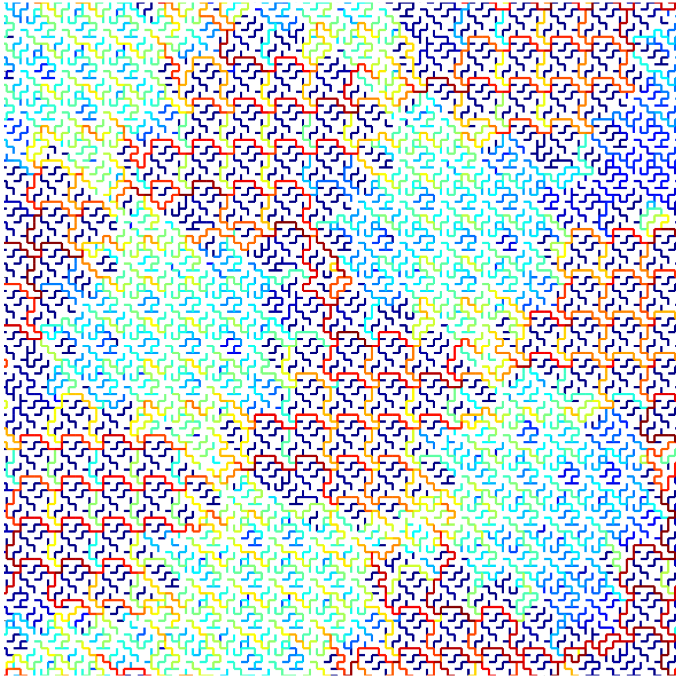
$$\begin{pmatrix} x' \\ y' \end{pmatrix} = r \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

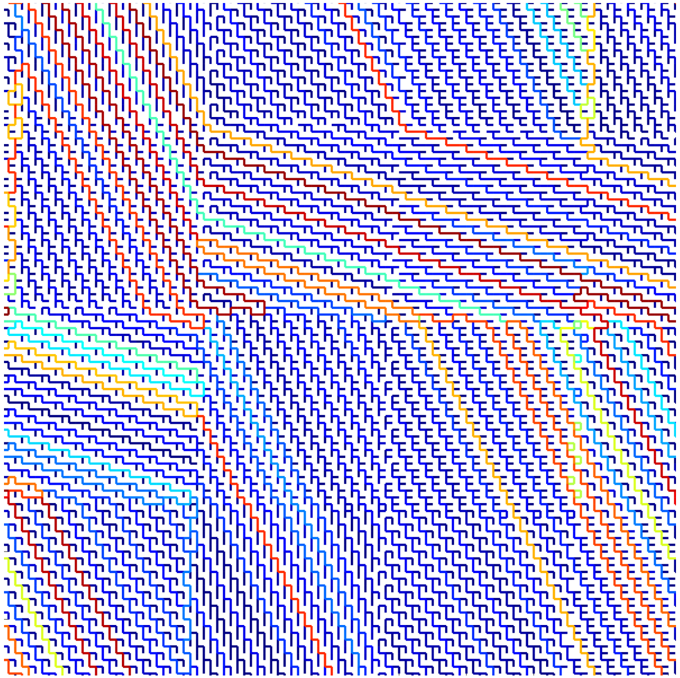
$$\psi\left(x', y'\right) = \cos 2\pi x' \cos 2\pi y'$$

$$\chi = \begin{cases} 1, & \psi \geq 0 \\ 0, & \psi < 0 \end{cases}$$

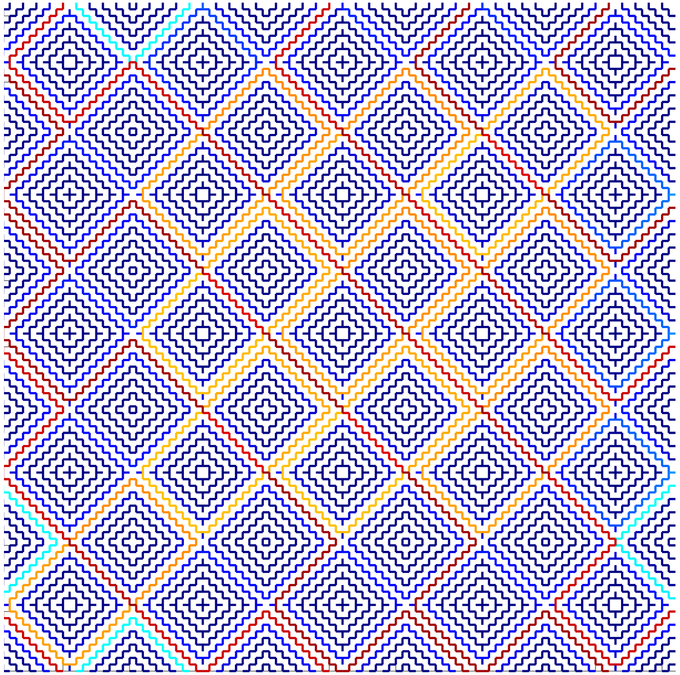
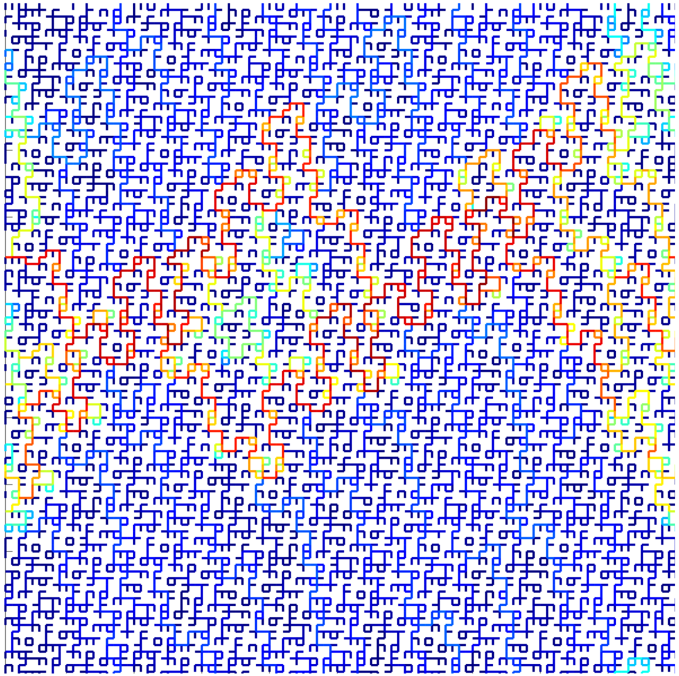
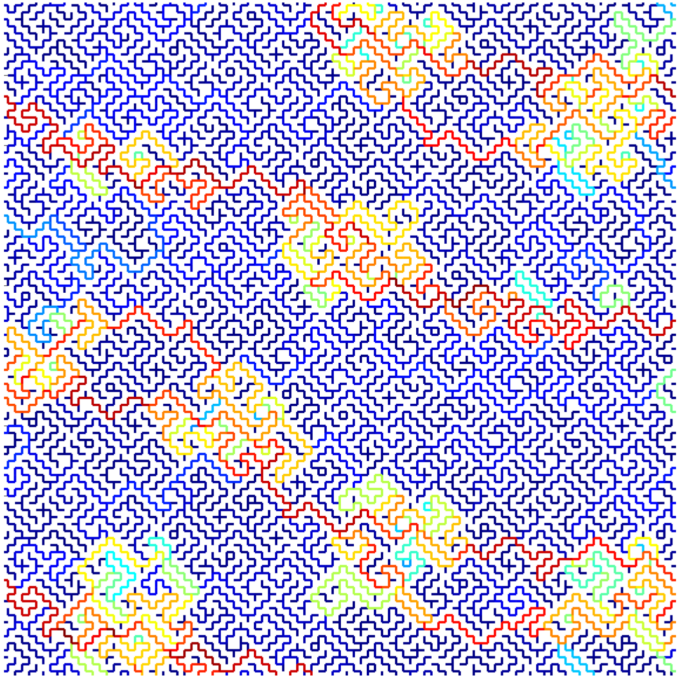
Wide Variety of Microgeometry





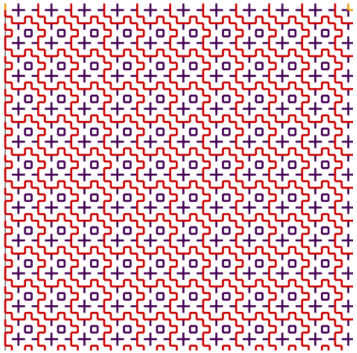


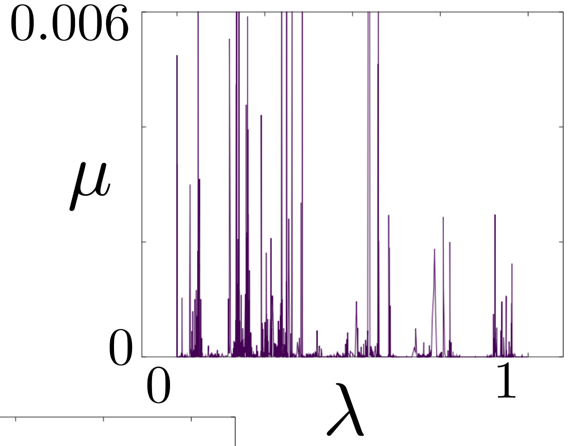
Wide Variety of Microgeometry

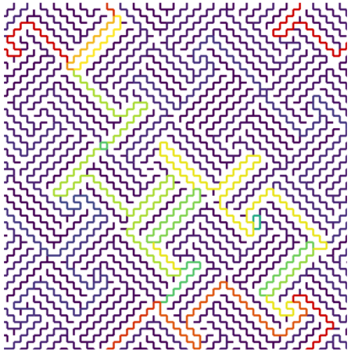




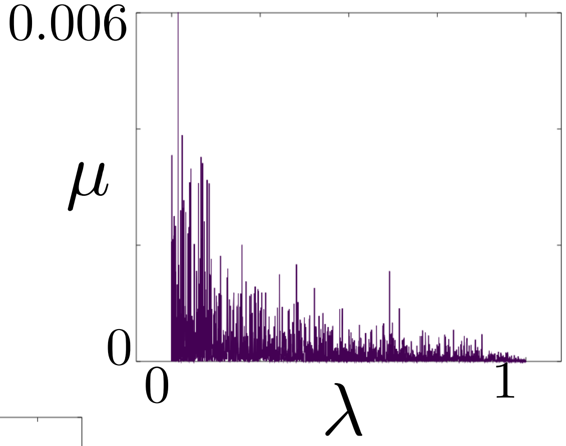
Periodic vs Aperiodic

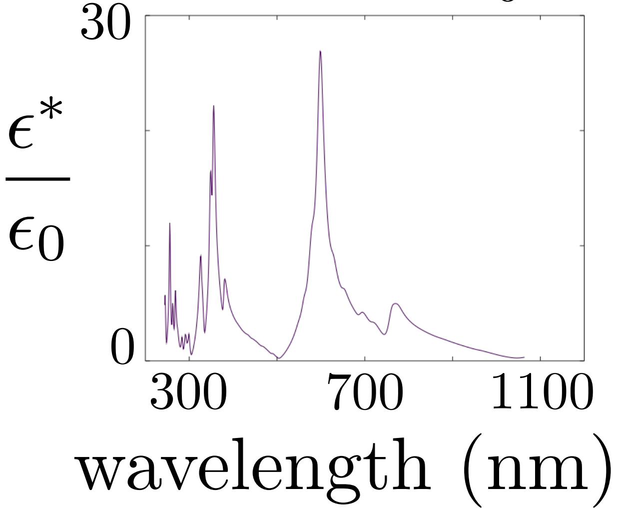
Dramatically Different Material Properties

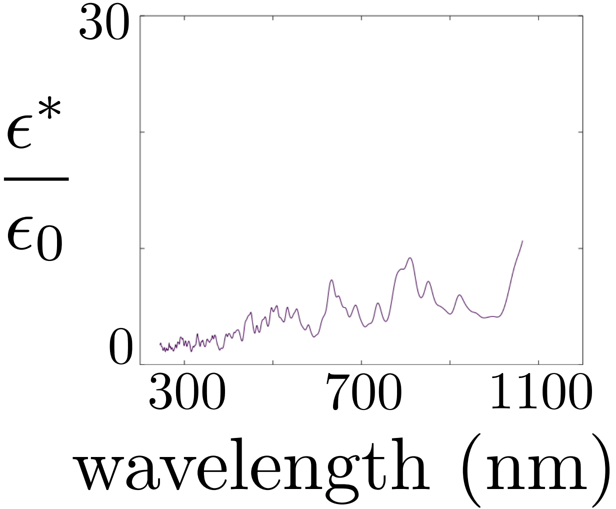






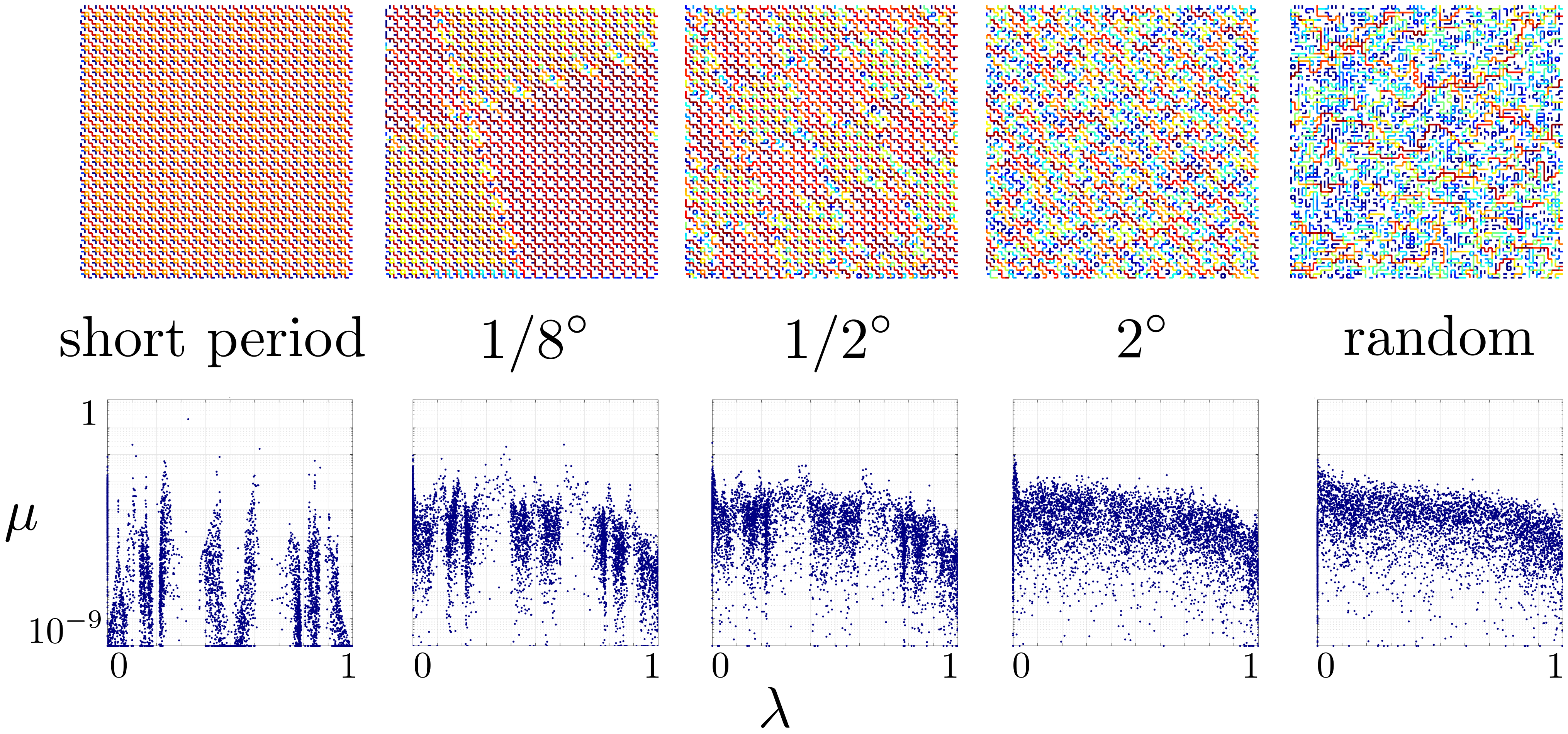






Optical dielectric function of gold
Olomon 2012
Phys. Rev. B

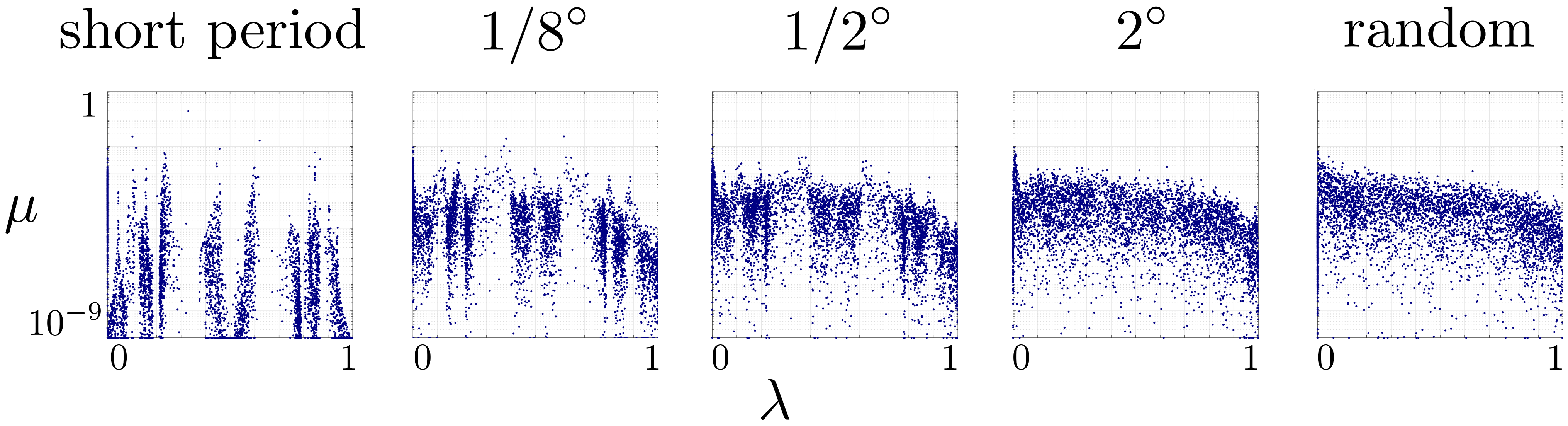
A Parameterized Transition



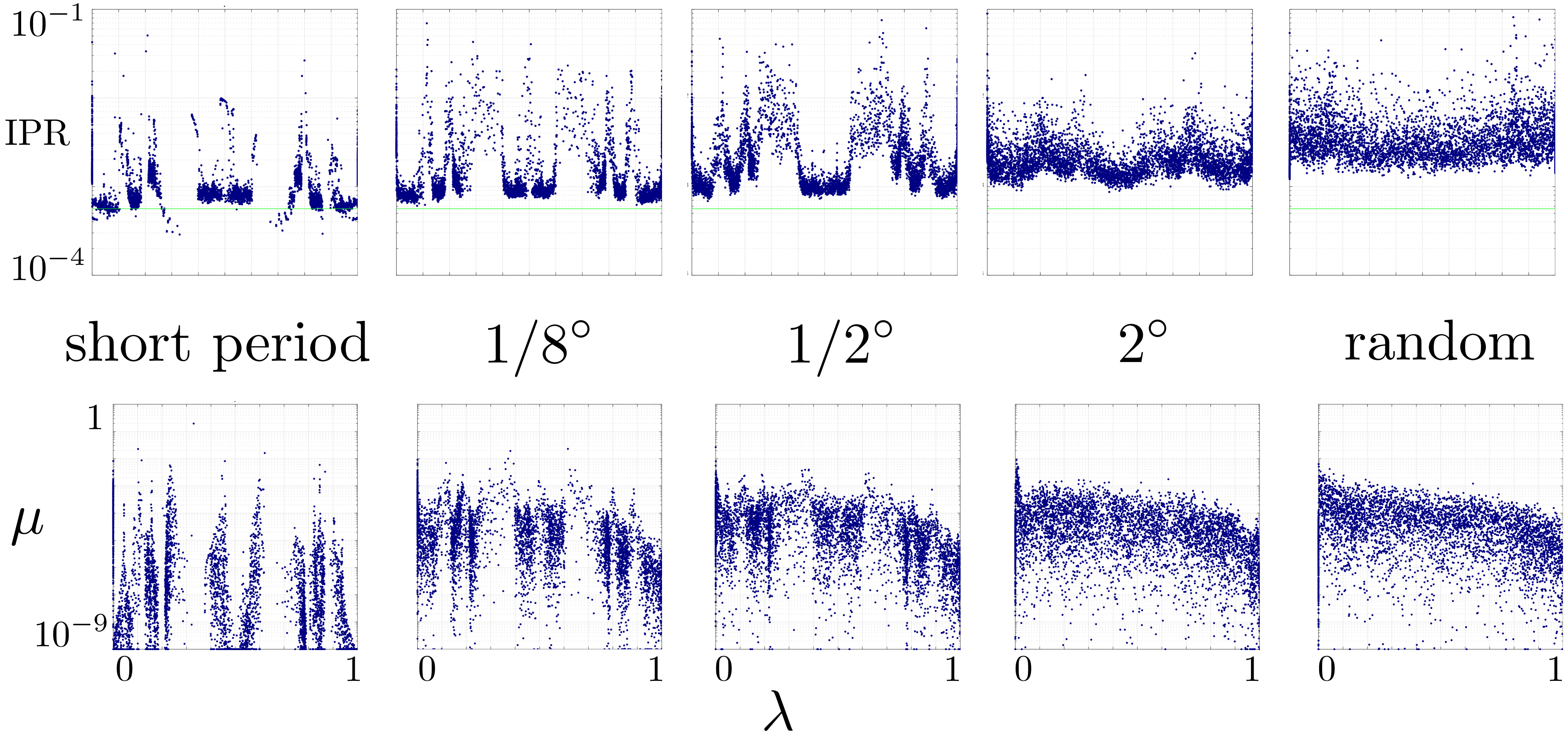
A Parameterized Transition

The inverse participation ration (IPR) summarizes the extended or localized nature of eigenvectors or distributions.

$$\mathrm{IPR}\left(\vec{x}\right) = \sum_i |x_i|^4$$



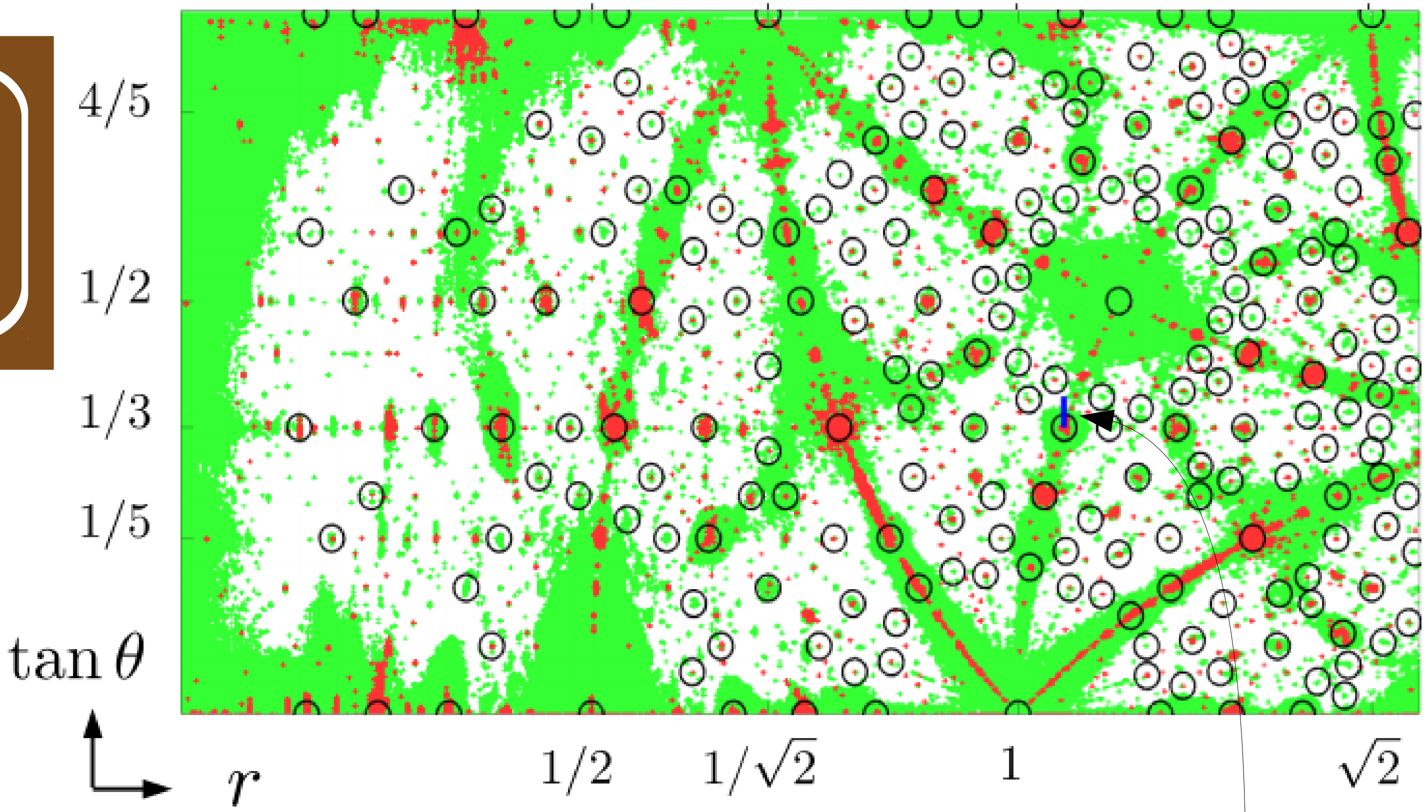
A Parameterized Transition



resonances **AND**
very extended states

resonances **XOR**
very extended states

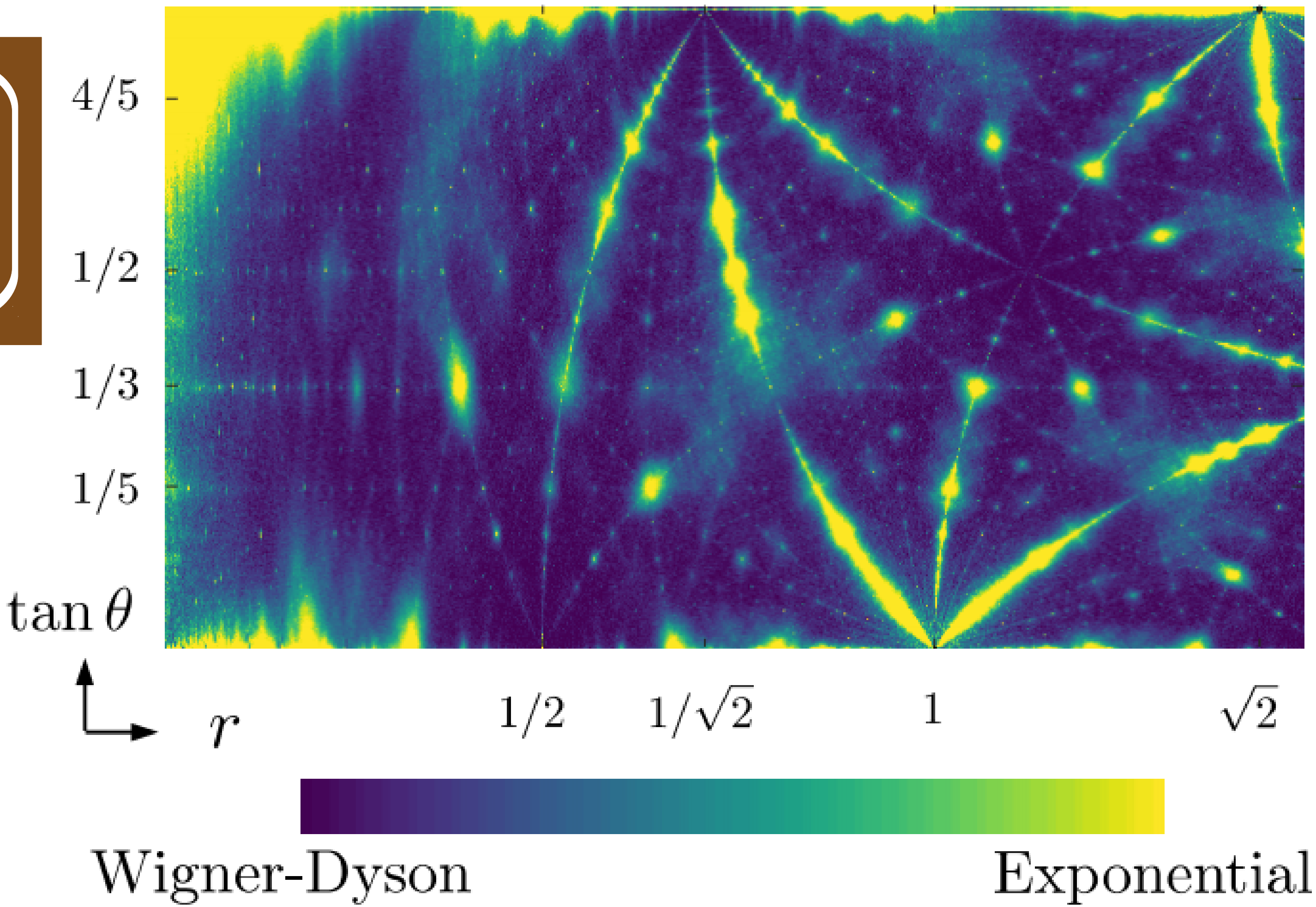
random like
material properties



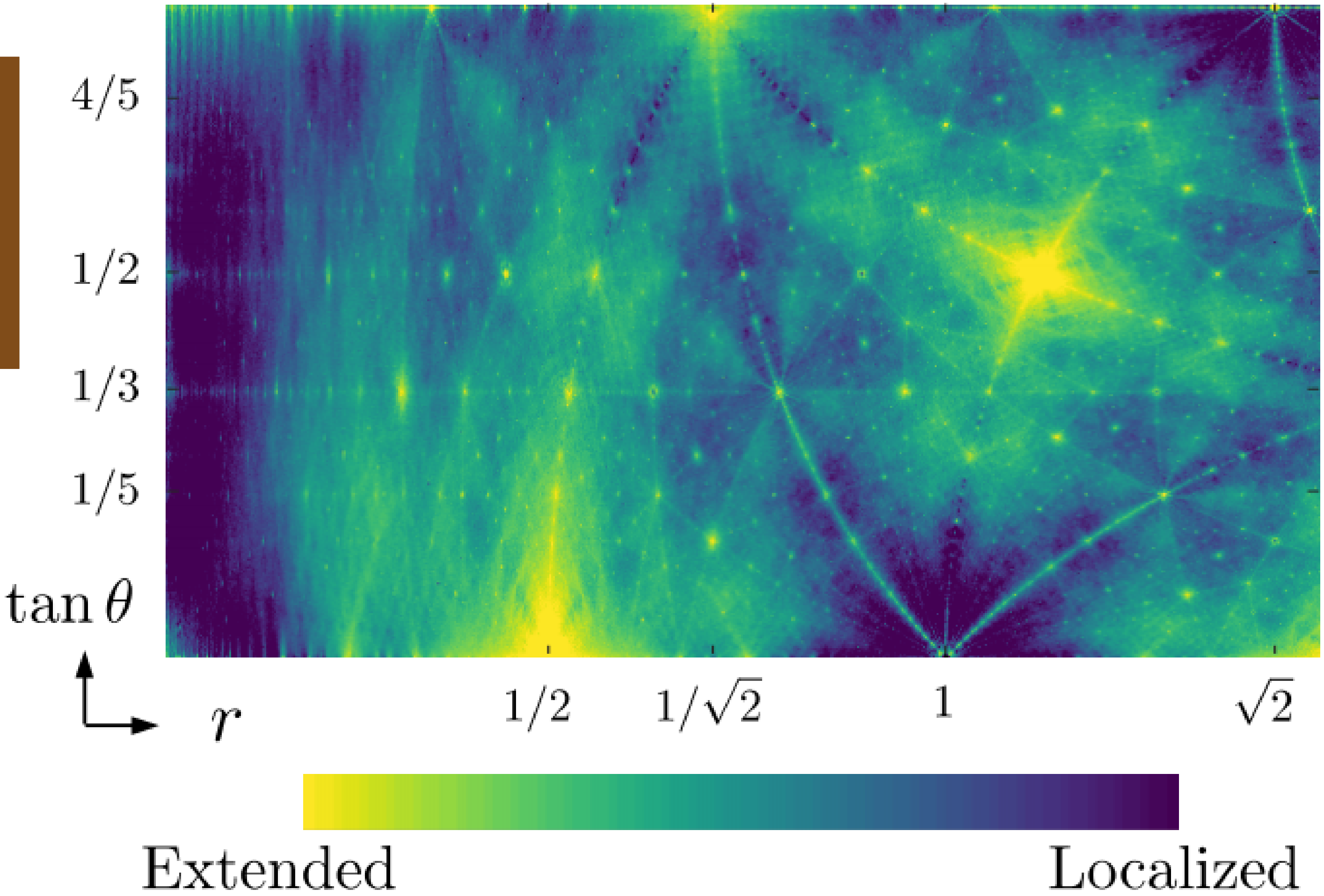
black circles ○ indicate
short period system geometry

We were here.


Scenic
Overview


4/5
1/2
1/3
1/5
tan θ
r
1/2
1/√2
1
√2
Wigner-Dyson
Exponential


Scenic
Overview


4/5
1/2
1/3
1/5
tan θ
r
1/2
1/√2
1
√2
Extended
Localized

Thank you for your time!