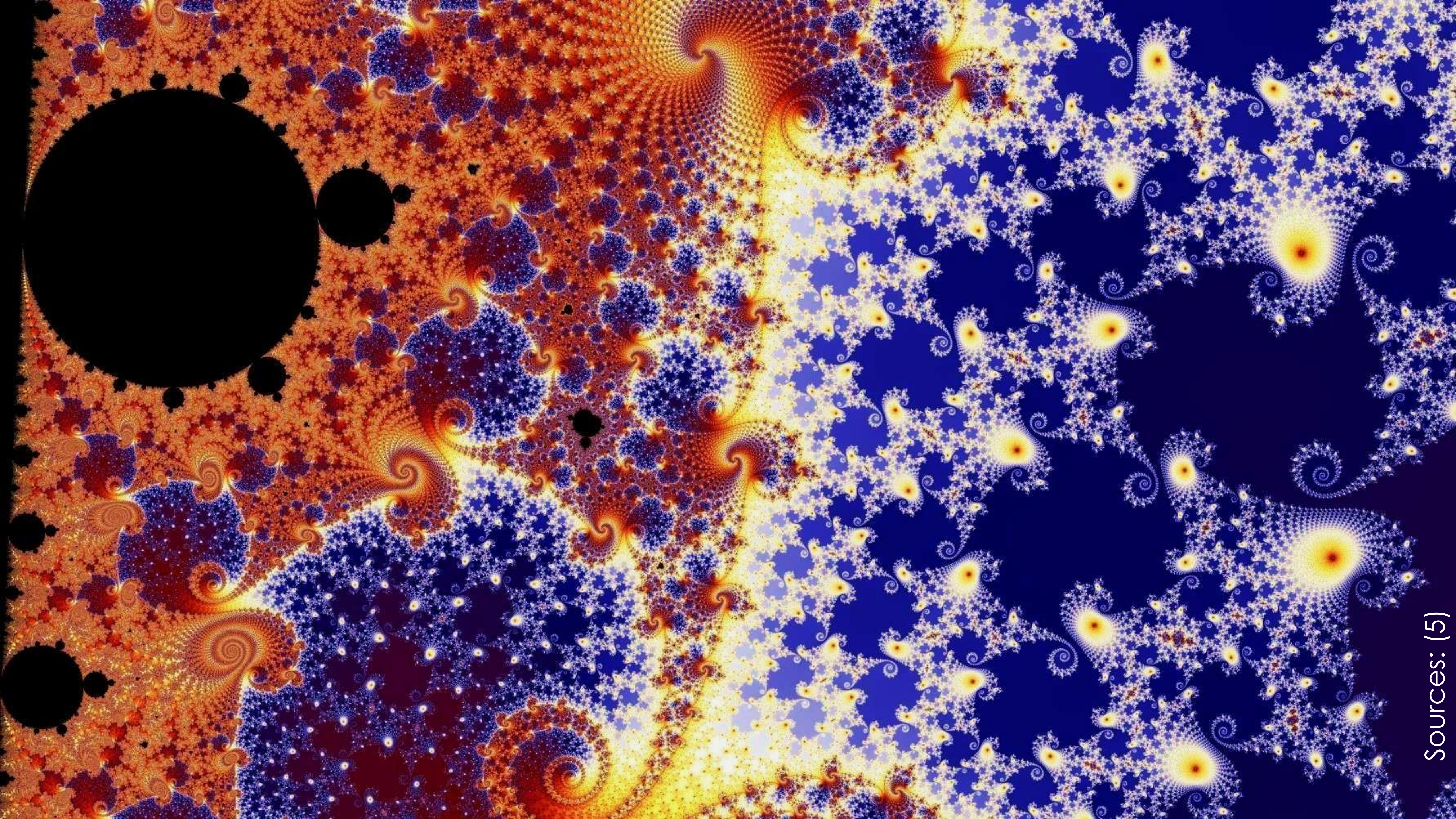


Sources: (5)

Fractals in AMO Physics

Maximilian Winterer
Your Passion For Physics – 23.11.2021
University Heidelberg

Outline

- Introduction to Fractals
- Fractional QM
  - Brownian Motion vs Lévi Flight Process
  - Results
  - Applications
- Outlook

What is a Fractal?

- ‘A rough or fragmented geometric shape that can be split into parts, each of which is a reduced-size copy of the whole’

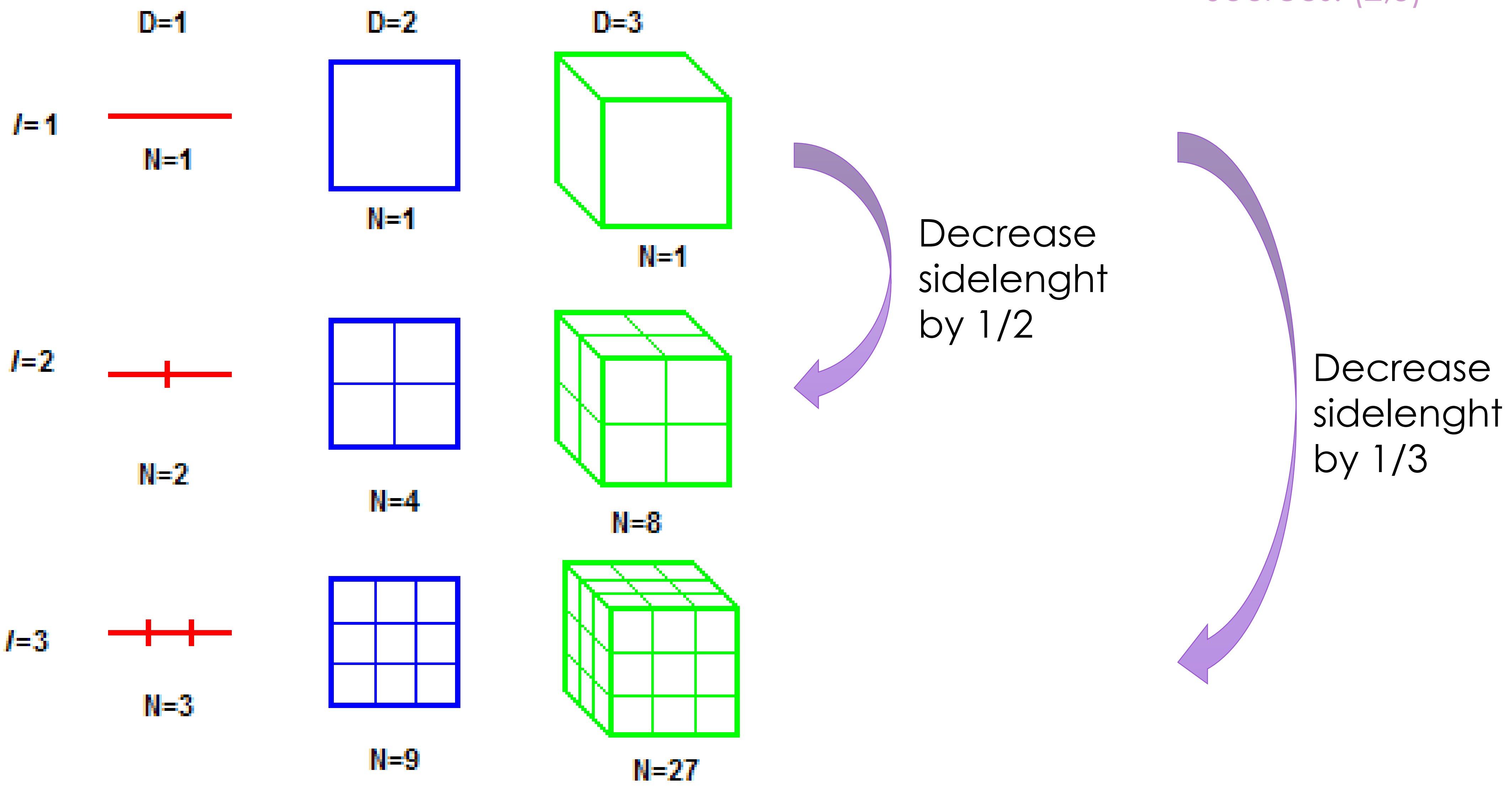
  ~ Benoît Mandelbrot

What is a Fractal?

- ‘A rough or fragmented geometric shape that can be split into parts, each of which is a reduced-size copy of the whole’
  ~ Benoît Mandelbrot
- Correct, but not what we are aiming for
  - Measure for roughness of objects when looking closer

  => Fractal Dimension

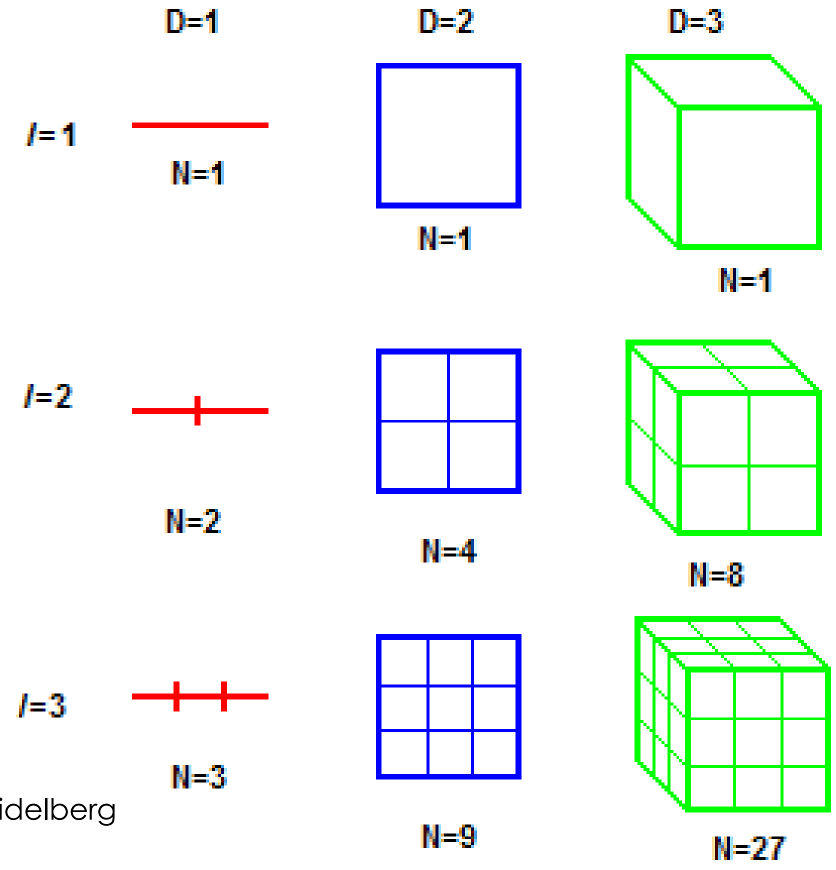
Sources: (2,3)


D=1
D=2
D=3
l=1
N=1
N=1
N=1
l=2
N=2
N=4
N=8
l=3
N=3
N=9
N=27
Decrease sidelenght by 1/2
Decrease sidelenght by 1/3

Fractal Dimension

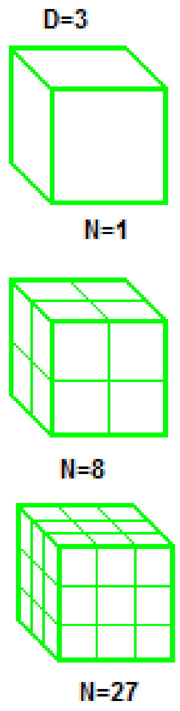
- Assign mass to each object (not formal, but intuitive derivation)

=> How does the mass scale?



Fractal Dimension

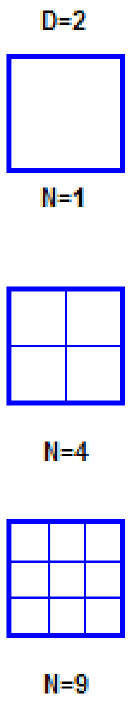
Relative Sidelength	Relative Mass
1	1
$\frac{1}{2}$	$\frac{1}{8} = \left(\frac{1}{2}\right)^3$
$\frac{1}{3}$	$\frac{1}{27} = \left(\frac{1}{3}\right)^3$



Sources: (2,3)

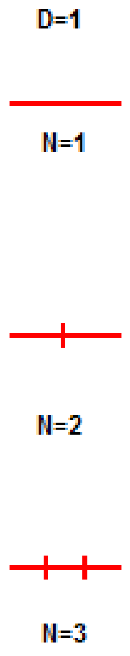
Fractal Dimension

Relative Sidelength	Relative Mass
1	1
$\frac{1}{2}$	$\frac{1}{4} = \left(\frac{1}{2}\right)^2$
$\frac{1}{3}$	$\frac{1}{9} = \left(\frac{1}{3}\right)^2$



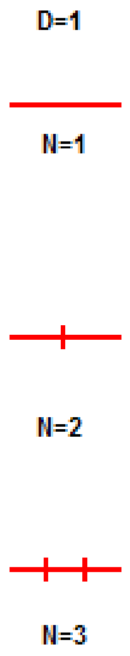
Fractal Dimension

Relative Sidelength	Relative Mass
1	1
$\frac{1}{2}$	$\frac{1}{2} = \left(\frac{1}{2}\right)^1$
$\frac{1}{3}$	$\frac{1}{3} = \left(\frac{1}{3}\right)^1$



Fractal Dimension

Relative Sidelength	Relative Mass
Dimension of Object	
$\frac{1}{2}$	$\frac{1}{2} = \left(\frac{1}{2}\right)^{1}$
$\frac{1}{3}$	$\frac{1}{3} = \left(\frac{1}{3}\right)^{1}$



Fractal Dimension – Sierpinski Triangle

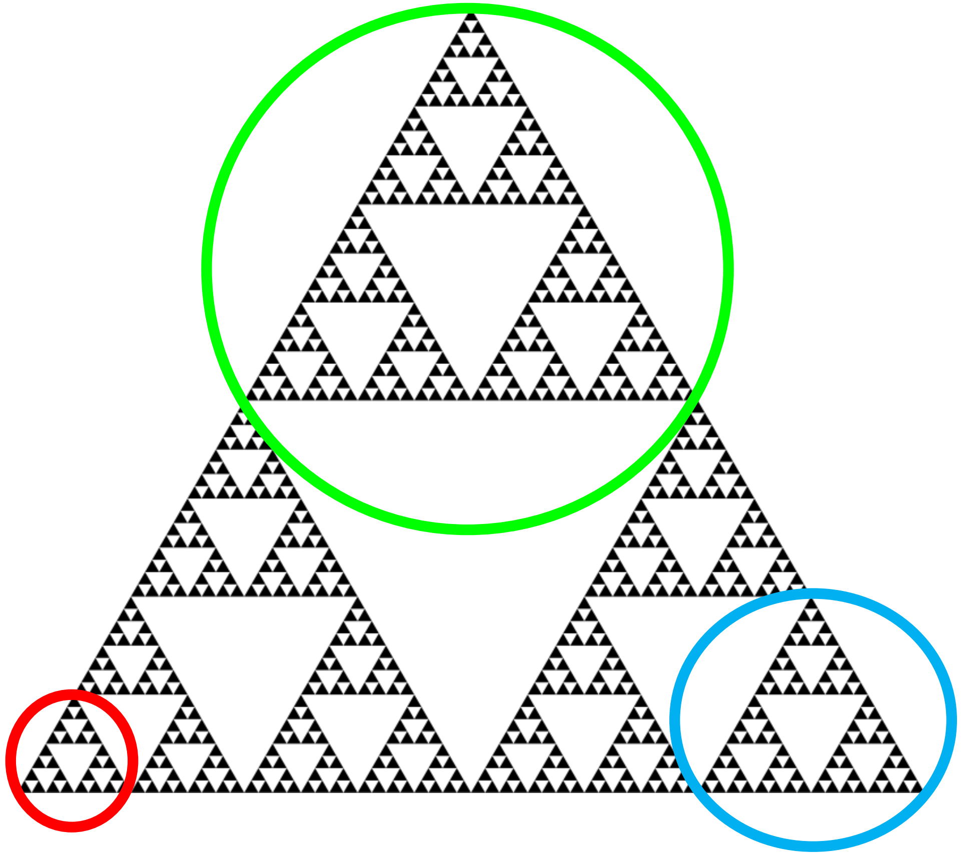
- Scale sidelenght by $\frac{1}{2}$

  => 'Mass' scales by $\frac{1}{3} = \left(\frac{1}{2}\right)^{?}$

  => $? = \frac{\log(3)}{\log(2)} = \log_2(3) = 1{,}584962 \ldots$

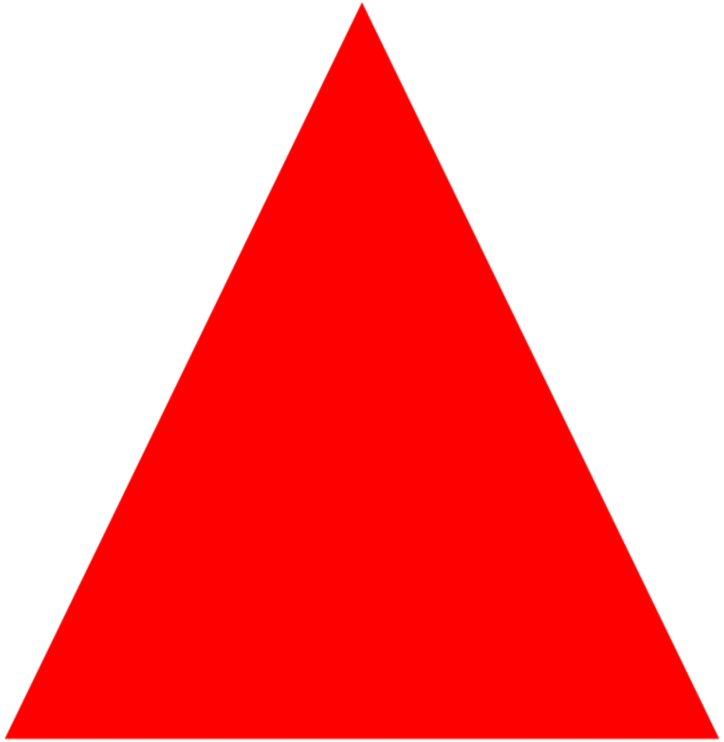
⇒ **Fractal Dimension:**

How much more detail can
I see when I zoom in/ when my
resolution increases?



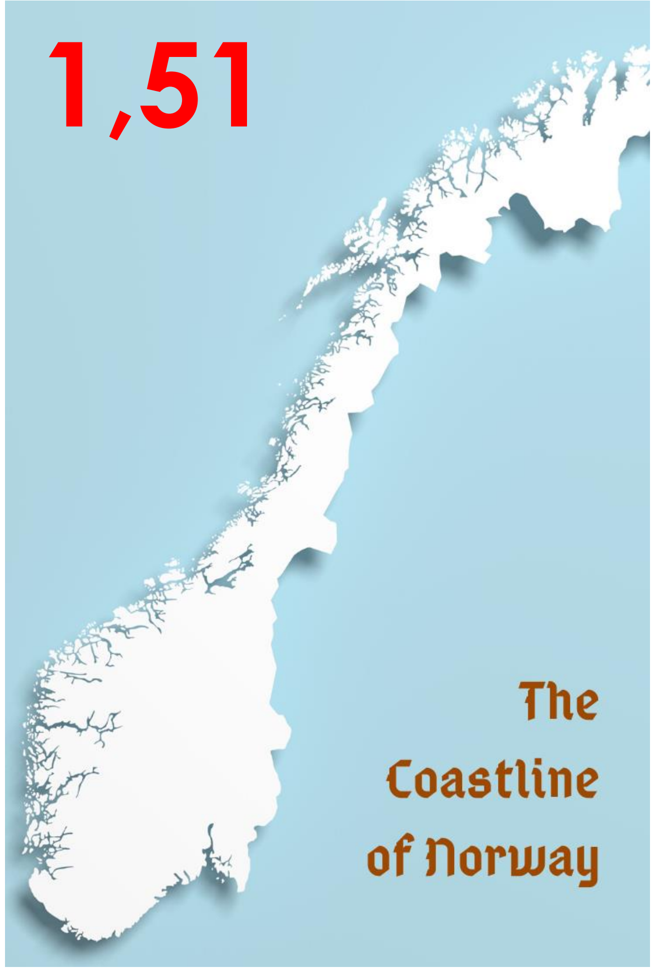
Fractal Dimension – Sierpinski Triangle

- Why is a ‚Fractal Dimension‘ necessary?



$$length = \infty$$
$$area = 0$$

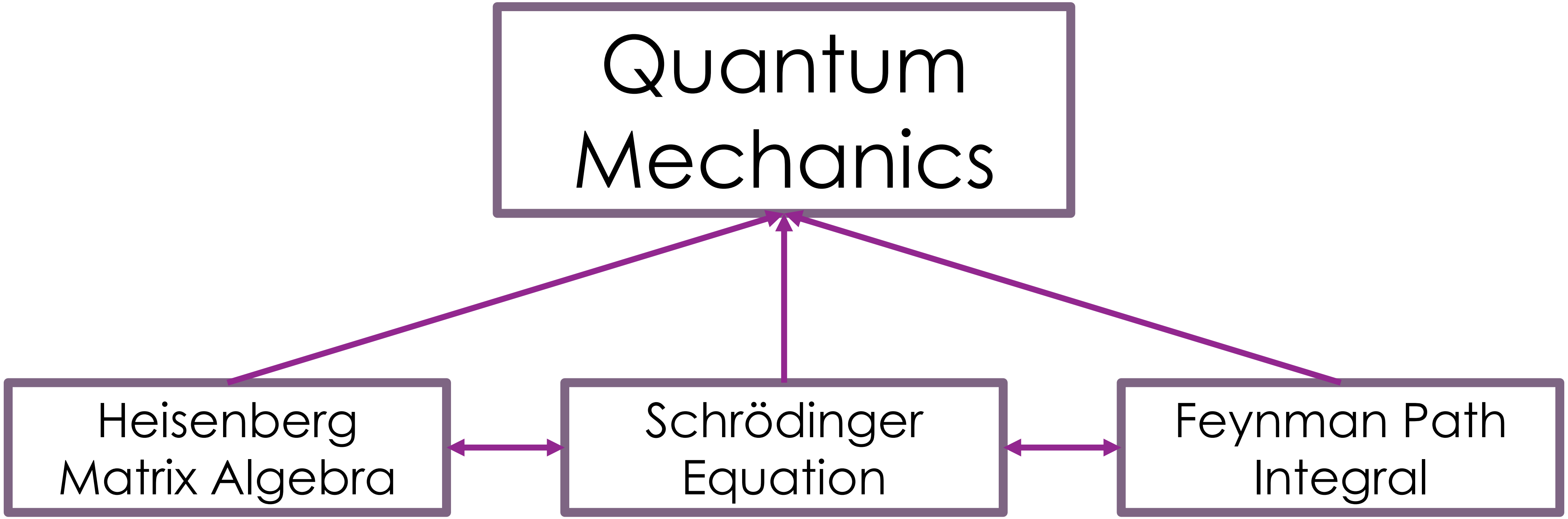
Why would one care about Fractals?



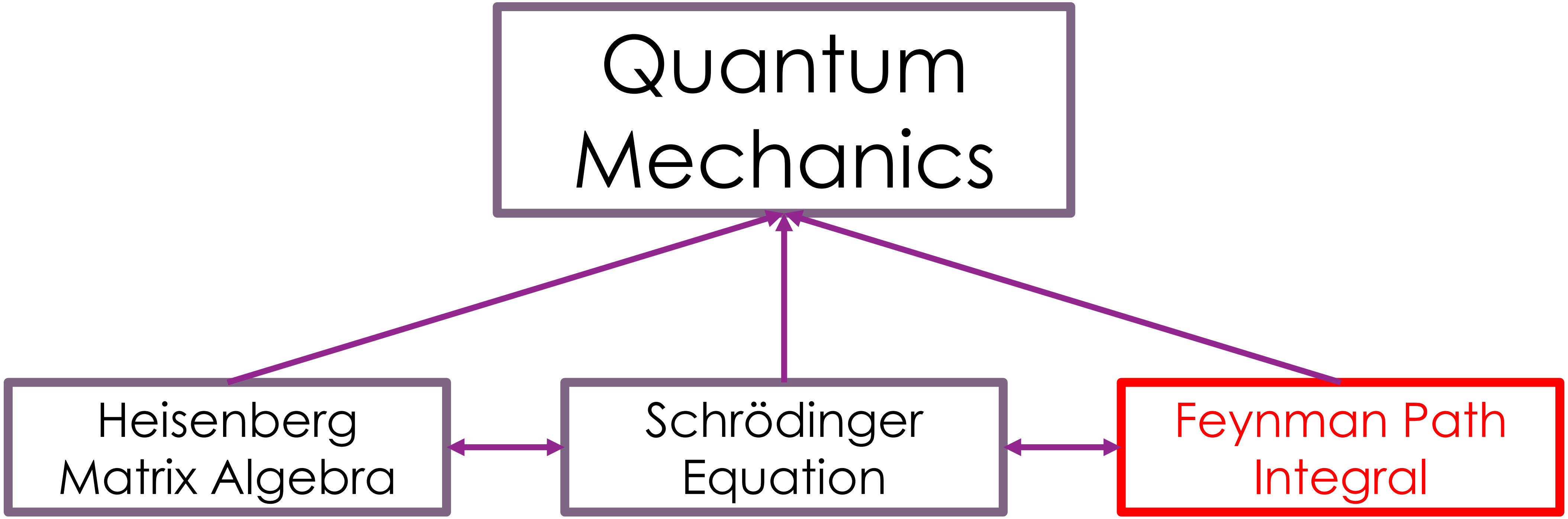
Questions?

Sources: (9,10)

Fractional Quantum Mechanics



Fractional Quantum Mechanics



Sources: (7,8,9,10)

Fractional Quantum Mechanics

- **Feynman Path Integral:** Integrates over all Brownian Paths from Initial State to Final State
- **Recap Brownian Path:** Trajectory following the **Brownian Motion** (Normal Distribution)
- **Generalized Motion:** **Lévi Flight** (Normal Distribution → Lévi Distribution)

Fractional Quantum Mechanics

- **Lévi Flight** (Normal Distribution → Lévi Distribution)
  - Probability Density Function (heavy-tailed):

$$f(x;\mu,c)=\sqrt{\frac{c}{2\pi}}\,\frac{e^{-\frac{c}{2(x-\mu)}}}{(x-\mu)^{3/2}}$$

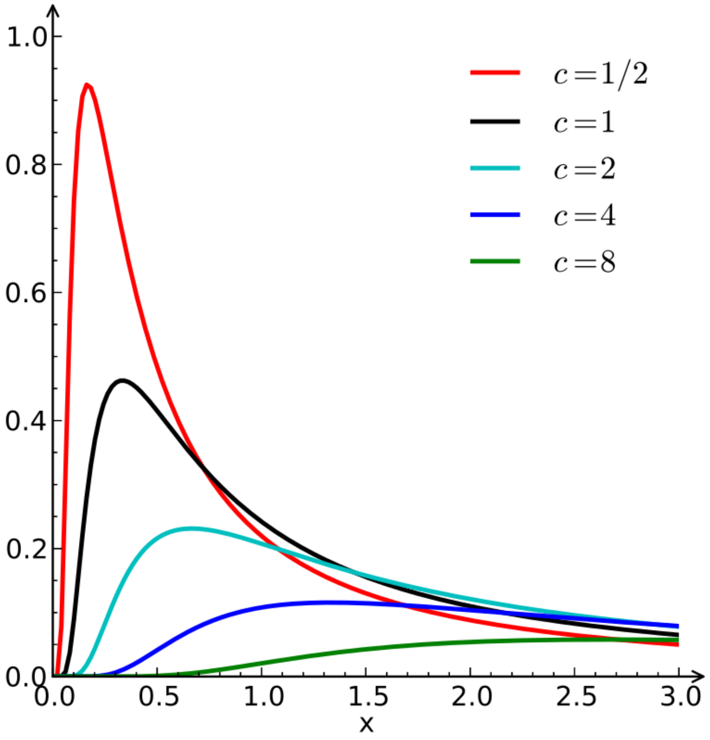
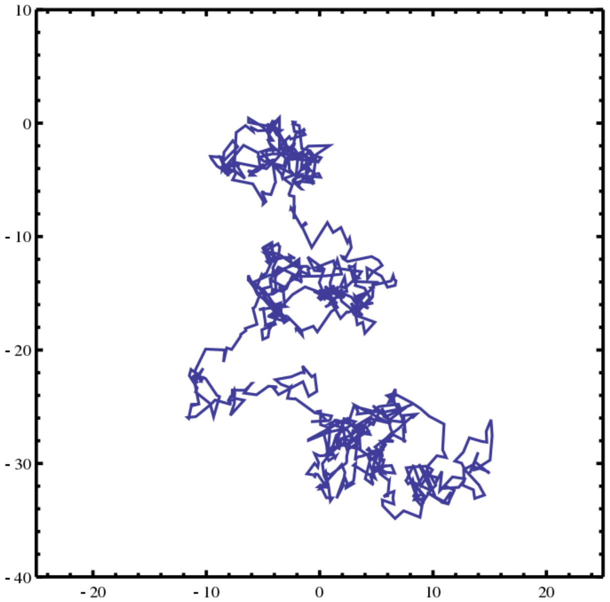


Figure 1: Probabilty Density function for a Lévi Distribution with different parameters c

Fractional Quantum Mechanics

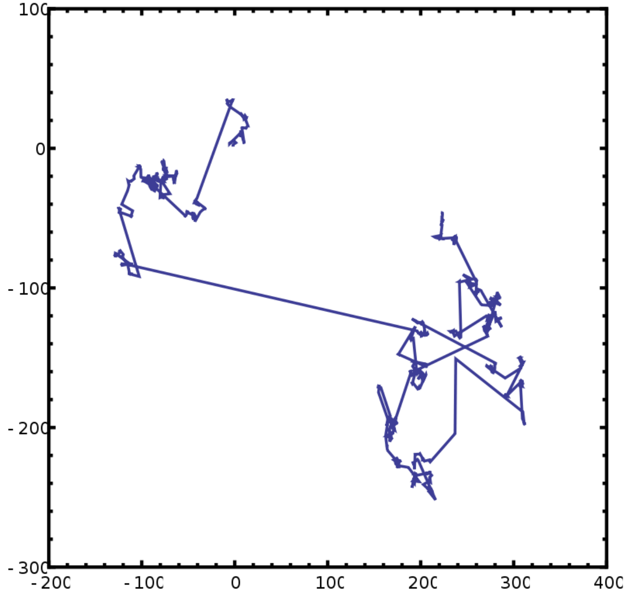
- **Lévi Flight**

Figure 2: Lévi Flight Trajectories for different Stability Parameters α



$\alpha = 2$
(Normal Distribution)

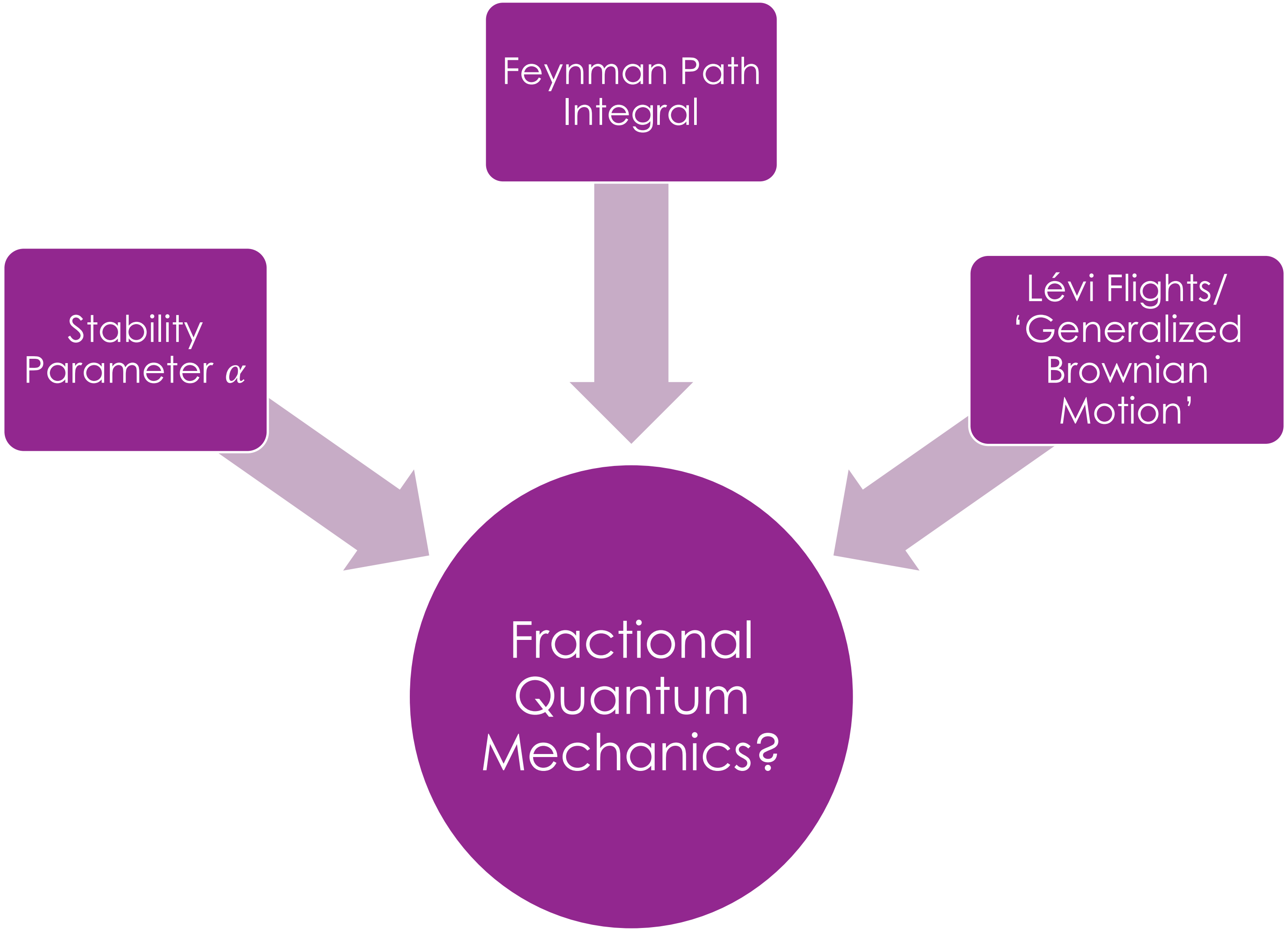
$\alpha = 1$
(Cauchy Distribution)



$\Rightarrow$ Lévi Index/ Stability Parameter α ‘defines’ path

$\Rightarrow$ Lévi Flights are self-similar (Fractals!)

Sources: (9,10)


Feynman Path Integral
Stability Parameter α
Lévi Flights/ ‘Generalized Brownian Motion’
Fractional Quantum Mechanics?

Fractional Quantum Mechanics

- Feynman Path Integral over Brownian Paths → Quantum Mechanics
- **Feynman Path Integral** over **Lévi Flights** → **Fractional Quantum Mechanics**
- **Stability Parameter** $\boldsymbol{\alpha}$ → **Fractal Dimension** $\boldsymbol{\alpha}$ (with $0 < \alpha \leq 2$)
- **Fractal Dimension** $\boldsymbol{\alpha}$ characterizes **Fractional Quantum Mechanics**

Fractional Quantum Mechanics

- Dispersion Relation for Fractional Quantum Mechanical Particle:

$$E_p = D_\alpha |p|^\alpha$$

- Fractional Schrödinger Equation:

$$i\hbar \frac{\partial \psi}{\partial t} = H_\alpha \psi$$

- Fractional Hamiltonian:

$$H_\alpha = -D_\alpha (\hbar \nabla)^\alpha + V(x)$$

Sources: (9,10)

Fractional Quantum Mechanics

$\Rightarrow$ Set $\alpha = 2$ $\rightarrow$ Brownian Motion Paths, Quantum Mechanics, Schrödinger Equation

$\Rightarrow$ Set $0 < \alpha < 2$ $\rightarrow$ Lévi Flight Paths, Fractional Quantum Mechanics, Fractional Schrödinger Equation

with α as Fractal Dimension

Applications of Fractional Quantum Mechanics

- Fractional systems reproduce well known QM systems when $\alpha \rightarrow 2$ (potential well, delta potential, oscillator, Bohr atom, …)
- Potential Realizations for Experimental Tests have been developed
- **One Experimental Result:**
  'The fractional symmetric rigid rotor' by Richard Herrmann in Journal of Physics G (2006)

Applications of Fractional Quantum Mechanics

- **'The fractional symmetric rigid rotor'**
  - Treat nuclids as rigid rotor
  - Use Fractional QM to calculate Eigenenergies (with $\alpha \neq 2$)

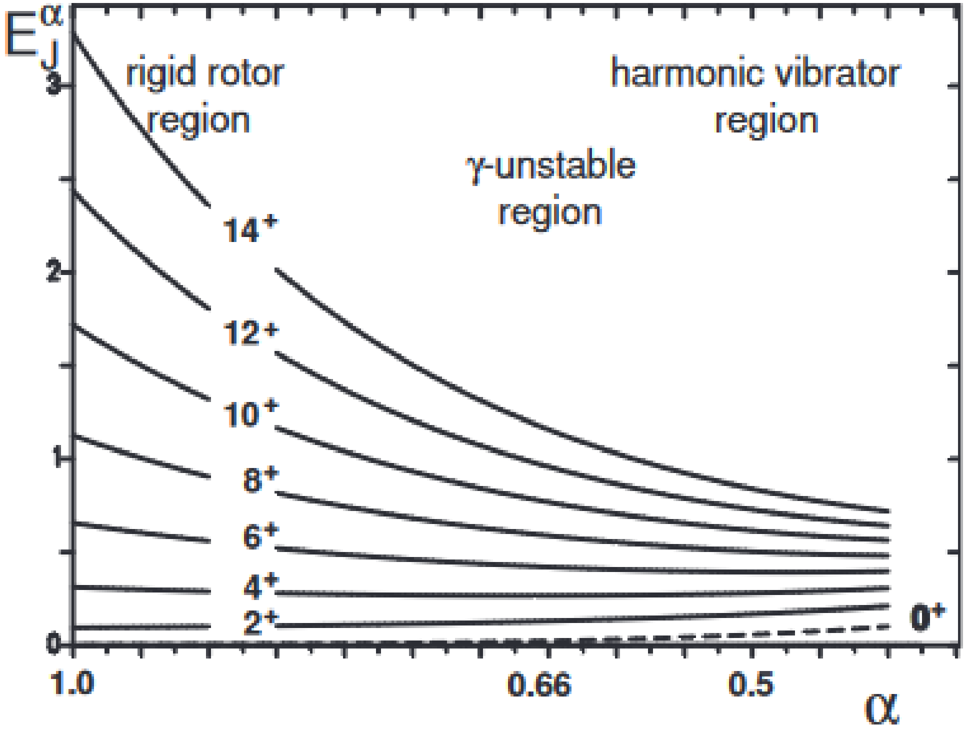


Figure 3: Eigenenergies of the Fractional Symmetric Rigid Rotor for different angular momenta J and different fractal dimensions α

Sources: (11)

Applications of Fractional Quantum Mechanics

- **'The fractional symmetric rigid rotor'**
  - ΔE mostly < 2%

nuclid	α	$a_0[keV]$	$m_0[keV]$	J_{max}	ΔE[%]
$^{156}_{92}Gd_{64}$	0.863	31.90	-43.65	14	2.23
$^{196}_{118}Pt_{78}$	0.710	175.06	-83.69	10	0.44
$^{110}_{62}Cd_{48}$	0.570	607.91	-405.80	6	0
$^{218}_{134}Po_{84}$	0.345	1035.69	-671.03	8	0.12
$^{164}_{88}Os_{76}$	0.624	339.423	-128.448	6	0
$^{170}_{94}Os_{76}$	0.743	125.128	-39.968	10	1.35
$^{172}_{96}Os_{76}$	0.767	89.010	-23.656	8	1.21
$^{174}_{98}Os_{76}$	0.771	63.388	-17.656	24	0.73
$^{176}_{100}Os_{76}$	0.808	51.231	-23.064	18	1.22
$^{178}_{102}Os_{76}$	0.816	49.882	-22.792	14	2.16
$^{180}_{104}Os_{76}$	0.841	45.309	-18.662	12	2.50
$^{182}_{106}Os_{76}$	0.903	32.002	-7.159	10	1.29
$^{184}_{108}Os_{76}$	0.904	31.690	-12.902	14	1.39
$^{186}_{110}Os_{76}$	0.882	40.433	-19.155	14	1.82
$^{188}_{112}Os_{76}$	0.875	44.567	-14.629	12	1.58
$^{190}_{114}Os_{76}$	0.847	58.055	-17.748	12	1.34
$^{192}_{116}Os_{76}$	0.835	63.774	-15.437	12	0.71
$^{214}_{126}Ra_{88}$	-0.007	374408	-376529	8	2.53
$^{214}_{126}Ra_{88}$	0.548	344.107	305.766	24	8.27
$^{216}_{128}Ra_{88}$	0.181	3665.36	-2887.88	10	4.22
$^{218}_{130}Ra_{88}$	0.536	321.622	-160.787	30	1.25
$^{220}_{132}Ra_{88}$	0.696	83.603	-25.966	30	0.26
$^{222}_{134}Ra_{88}$	0.831	33.221	-5.67	6	0
$^{224}_{136}Ra_{88}$	0.841	27.295	-8.849	12	1.57

Table 1: Root mean square errors ΔE between experimental data and predictions, and fitting parameters including Fractal Dimension α for different nuclids

Sources: (11)

Applications of Fractional Quantum Mechanics

- **'The fractional symmetric rigid rotor'**
  - ΔE mostly $< 2\%$

=> Result is **better** by **factor of 3 to 6** compared to results from **Taylor expansion** up to **second order** in J

nuclid	α	$a_0[keV]$	$m_0[keV]$	J_{max}	ΔE[%]
$^{156}_{92}Gd_{64}$	0.863	31.90	-43.65	14	2.23
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Table 1: Root mean square errors ΔE between experimental data and predictions, and fitting parameters including Fractal Dimension α for different nuclids

Summary

- **Fractals:**
  - Mandelbrot: Fractals = Self similar Objects
  - Fractal Dimension describes roughness of Object
  - Fractals describe **our** world without unnecessary simplifications
- **Fractional QM:**
  - Lévi Flights in Feynman Path Integral => Fractional QM
  - Result: Well known QM equations, but adjusted by Fractal Dimension
  - Potential Realizations were developed
  - Fractional Symmetric Rigid Rotor for heavy nuclides shows agreement

Outlook

- One Dimensional Lévi Crystal for further Tests
- Further Applications of Fractals:
  - Molecular Complexity/ Drug Discovery (Appendix)
  - Diffraction by an Optical Fractal Grating (Appendix)
  - Fractals and Chaotic Scattering of Atoms in the Field of a Standing Light Wave

Sources

(1) 'The Fractal Geometry of Nature', Benoît B. Mandelbrot, 1982

(2) https://en.wikipedia.org/wiki/Fractal_dimension

(3) https://www.youtube.com/watch?v=gB9n2gHsHN4

(4) https://en.wikipedia.org/wiki/Sierpi%C5%84ski_triangle

(5) Google Images

(6) 'Classification and dynamics of tropical clouds by their fractal dimension', Batista-Tomás

(7) https://en.wikipedia.org/wiki/L%C3%A9vy_flight

(8) https://en.wikipedia.org/wiki/L%C3%A9vy_distribution

(9) 'Fractional quantum mechanics', Nick Laskin, Physical Review E, 6th April 2000

(10) 'Fractional quantum mechanics', Nick Laskin (book), 2018

(11) 'The fractional symmetric rigid rotor', Richard Herrmann, Journal of Physics G, 15th September 2006

(12) 'Molecular Complexity Calculated by Fractal Dimension', Modest von Korff, Scientific Reports, 30th January 2019

(13) 'Diffraction by an optical fractal grating', Bo Hou, Applied Physics Letters, 20th December 2004

(14) 'Fractals and Chaotic Scattering of Atoms in the Field of a Standing Light Wave', V. Yu. Argonov, Journal of Experimental and Theoretical Physics, 25th November 2002

Questions?

Sources: (12)

Appendix: Molecular Complexity/ Drug Discovery

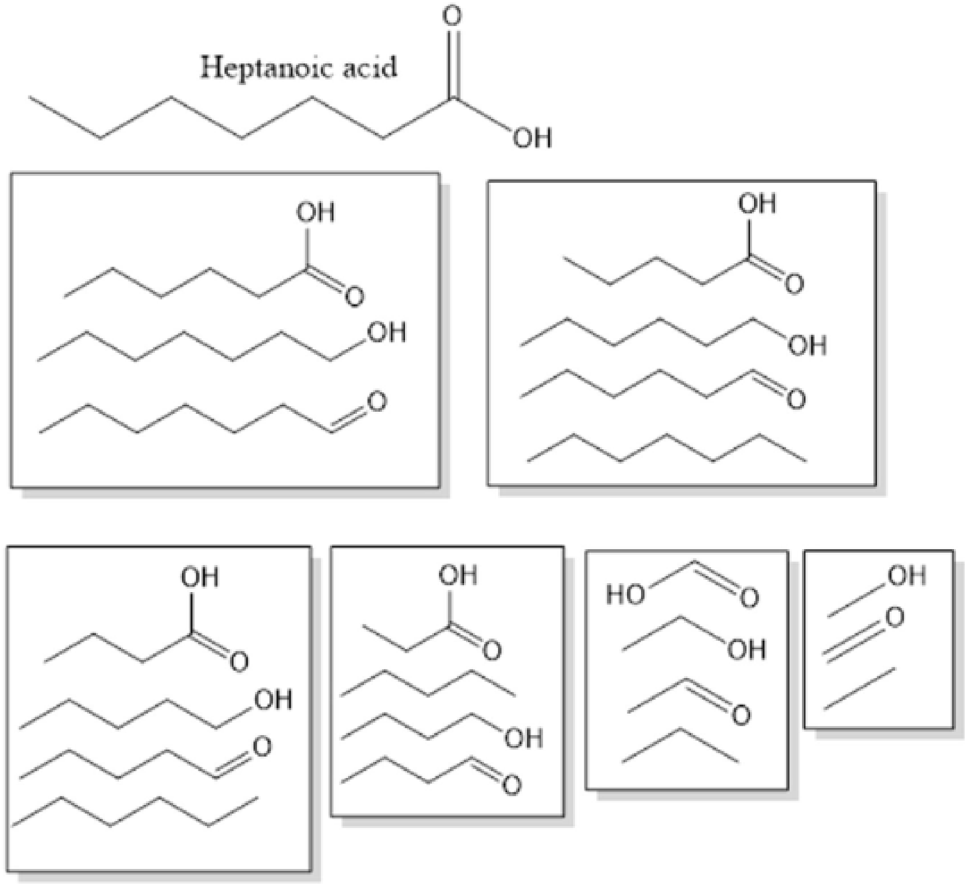


Figure 4: Heptanoic acid and its distinct substructures, grouped by bond counts

Appendix: Molecular Complexity/ Drug Discovery

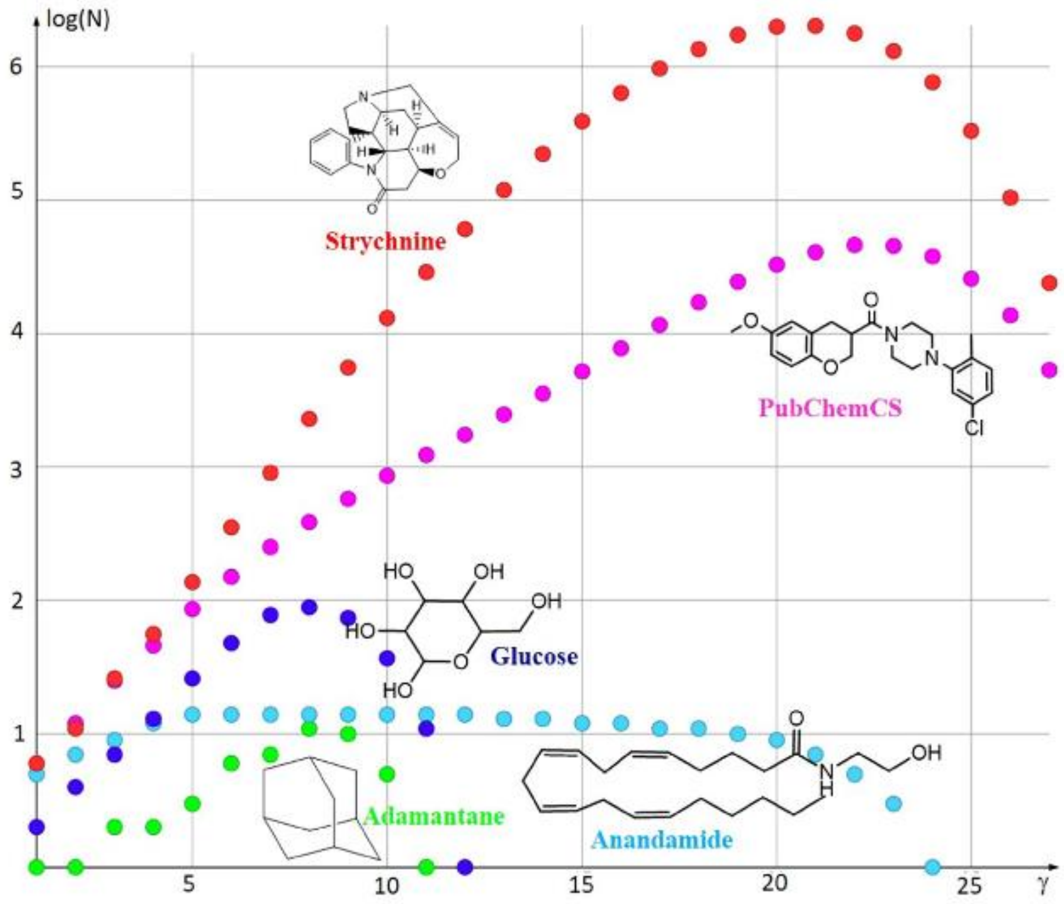


Figure 5: Number of distinct subgraphs in logarithmic scaling for five different example molecules over the bond count of the subgraphs

Sources: (12)

Appendix: Molecular Complexity/ Drug Discovery

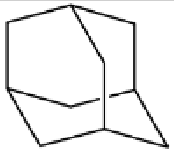
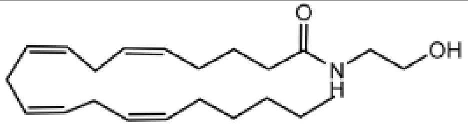
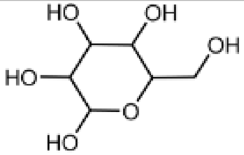
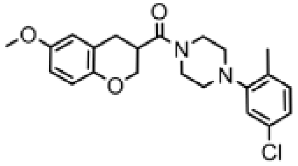
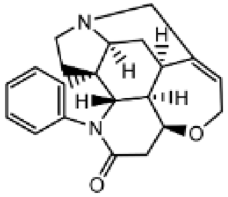
Name	Structure	N_{max}	γ_{max}	dim(M)
Adamantane		11	8	1.2
Anandamide		14	5	1.6
Glucose		89	8	2.2
PubChemCS		45,973	22	3.5
Strychnine		2,022,462	21	4.8

Table 2: The maximum number of distinct fragments N_{max}, the corresponding bond count γ_{max}, and the fractal dimension $\dim(M)$ of the five example molecules.

Appendix: Molecular Complexity/ Drug Discovery

Molecular complexity is an important characteristic of organic molecules for drug discovery. How to calculate molecular complexity has been discussed in the scientific literature for decades. It was known from early on that the numbers of substructures that can be cut out of a molecular graph are of importance for this task. However, it was never realized that the cut-out substructures show self-similarity to the parent structures. A successive removal of one bond and one atom returns a series of fragments with decreasing size. Such a series shows self-similarity similar to fractal objects. Here we used the number of distinct fragments to calculate the fractal dimension of the molecule. The fractal dimension of a molecule is a new matter constant that incorporates all features that are currently known to be important for describing molecular complexity. Furthermore, this is the first work that reveals the fractal nature of organic molecules.

Abstract of 'Molecular Complexity Calculated by Fractal Dimension' by Modest von Korff in Scientific Reports (30th January 2019)

Appendix: Diffraction by an Optical Fractal Grating

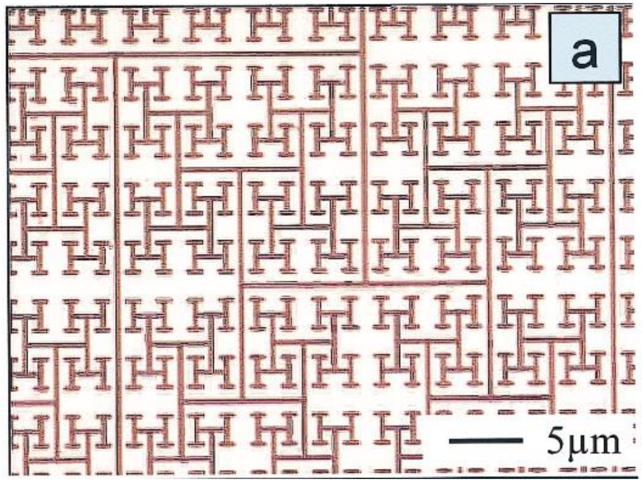
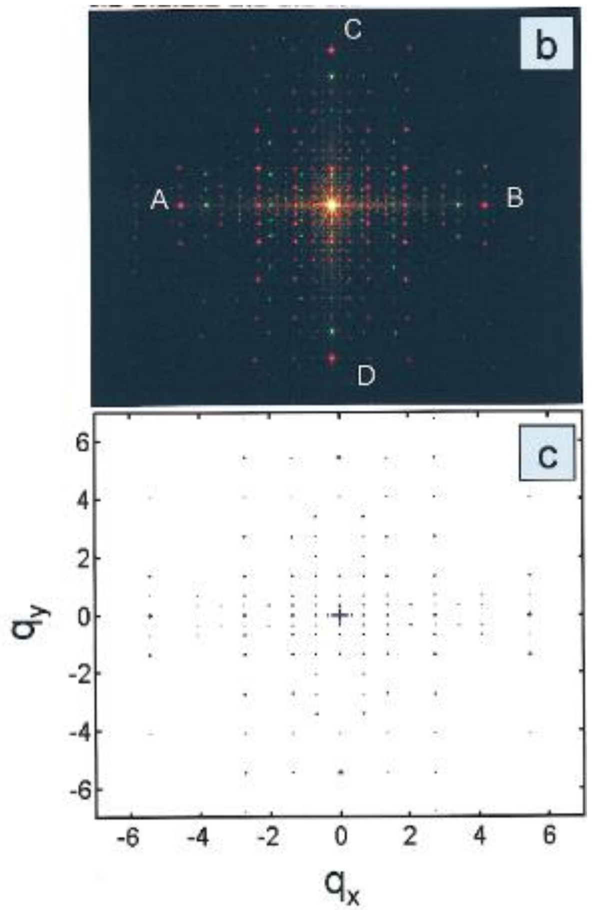


Figure 6:
(a) A part of the 15-level H-fractal grating
(b) The experimental Fraunhofer diffraction pattern under two illuminating wavelengths: 532 nm (green) and 633 nm (red)
(c) The calculated diffraction spectrum of the fractal grating.



Appendix: Diffraction by an Optical Fractal Grating

We report experimental and theoretical studies of Fraunhofer diffraction pattern of a 15-level H-fractal grating. The diffraction pattern was found to exhibit self-similarity. In particular, the diffracted light was found to be more intense at higher spatial frequencies than at lower frequencies, in stark contrast to the diffraction patterns of wire gratings and grid gratings. Using Fourier transform theory, we show that this unusual behavior comes from the structural coherence of the H-fractal, which makes it favorable to use higher-order diffraction spectra for larger dispersion. In addition, the fractal dimension of the grating is shown analytically and experimentally to be two. ©

Abstract of 'Diffraction by an optical fractal grating' by Bo Hou in Applied Physics Letters (20th December 2004)