HSRM Summer School 2016

Hilbert Space Methods in Quantum Mechanics

Prof. Dr. Detlef Lehmann

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Part I :

Part II :

1. The Double-Slit Experiment

- There are two basic physical phenomena:

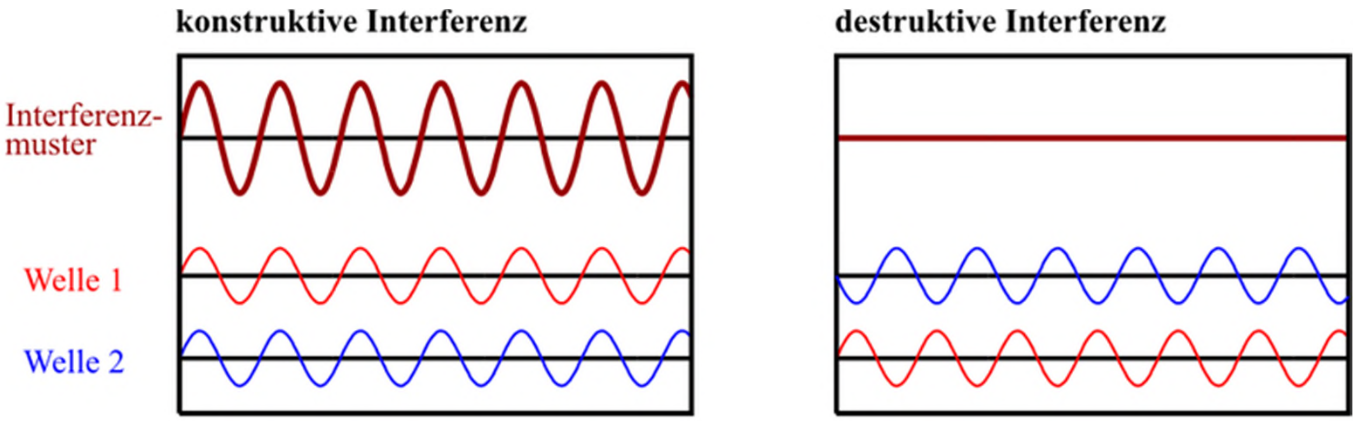
Particles and Waves

- Experiments have shown: On an atomic scale,

  - particles can behave like waves → double-slit experiment, electron diffraction
  - waves can behave like particles → photoelectric effect, Compton effect

1. The Double-Slit Experiment

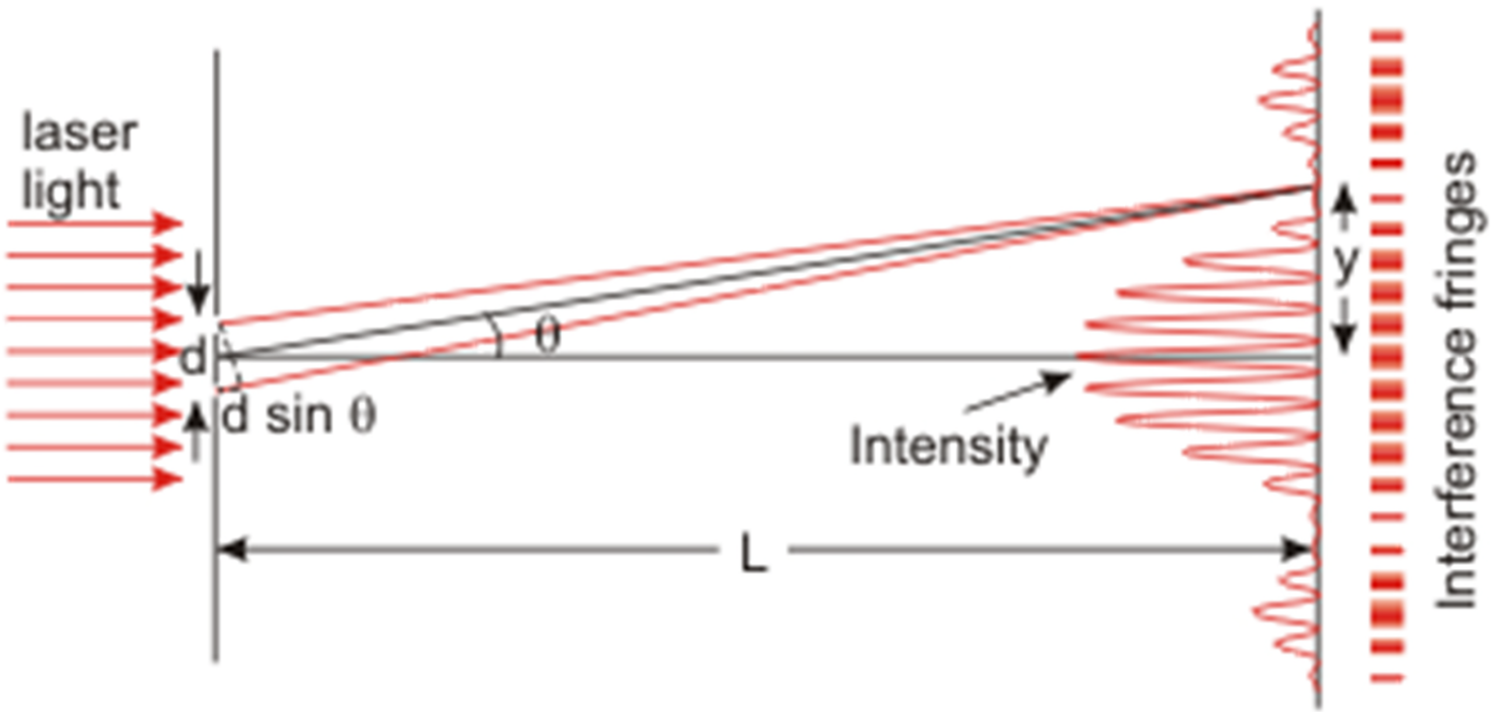
- Basic property of waves: they can interfere



- Experiments have shown: Electrons can also interfere .
- From a conceptual point of view, the double-slit experiment shows this in the most clean and transparent way.

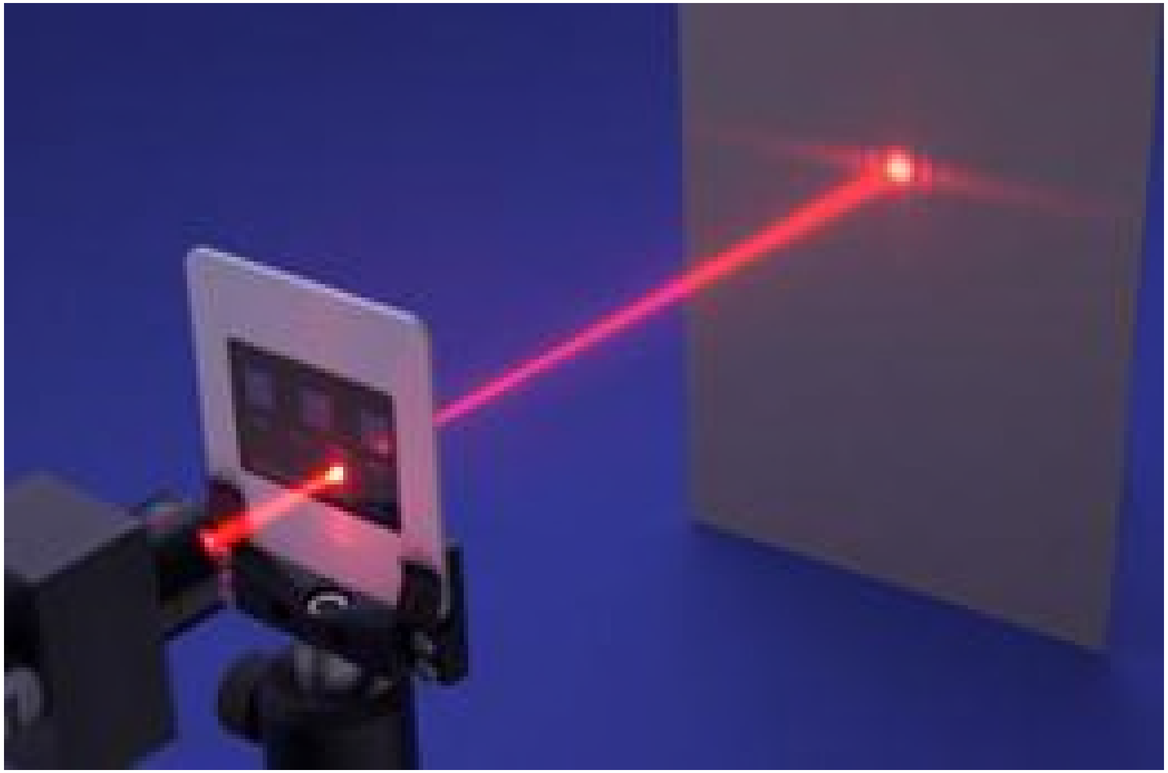
1. The Double-Slit Experiment

- Experimental setup:



1. The Double-Slit Experiment

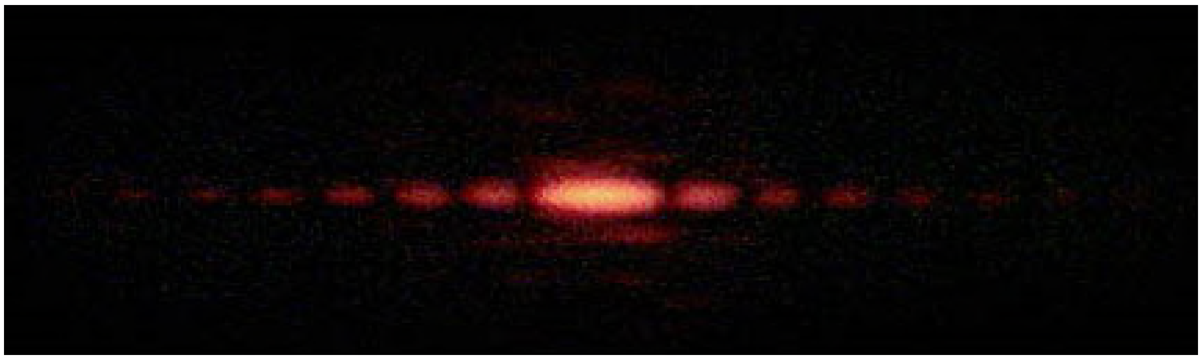
- Experimental setup: with laser light, this can be done at school



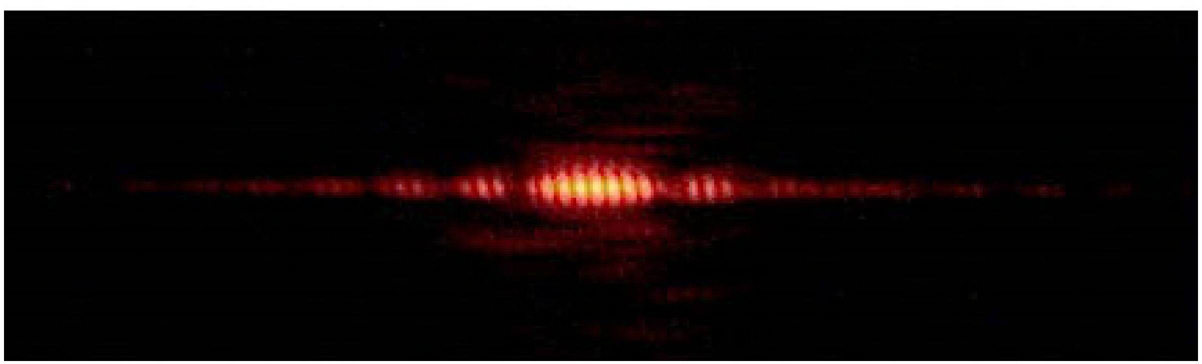
- With electrons, the actual setup is quite sophisticated (later more on this)

1. The Double-Slit Experiment

- the following interference pattern shows up: single-slit / double-slit :



Laser light passing through a single slit, showing basic diffraction pattern.



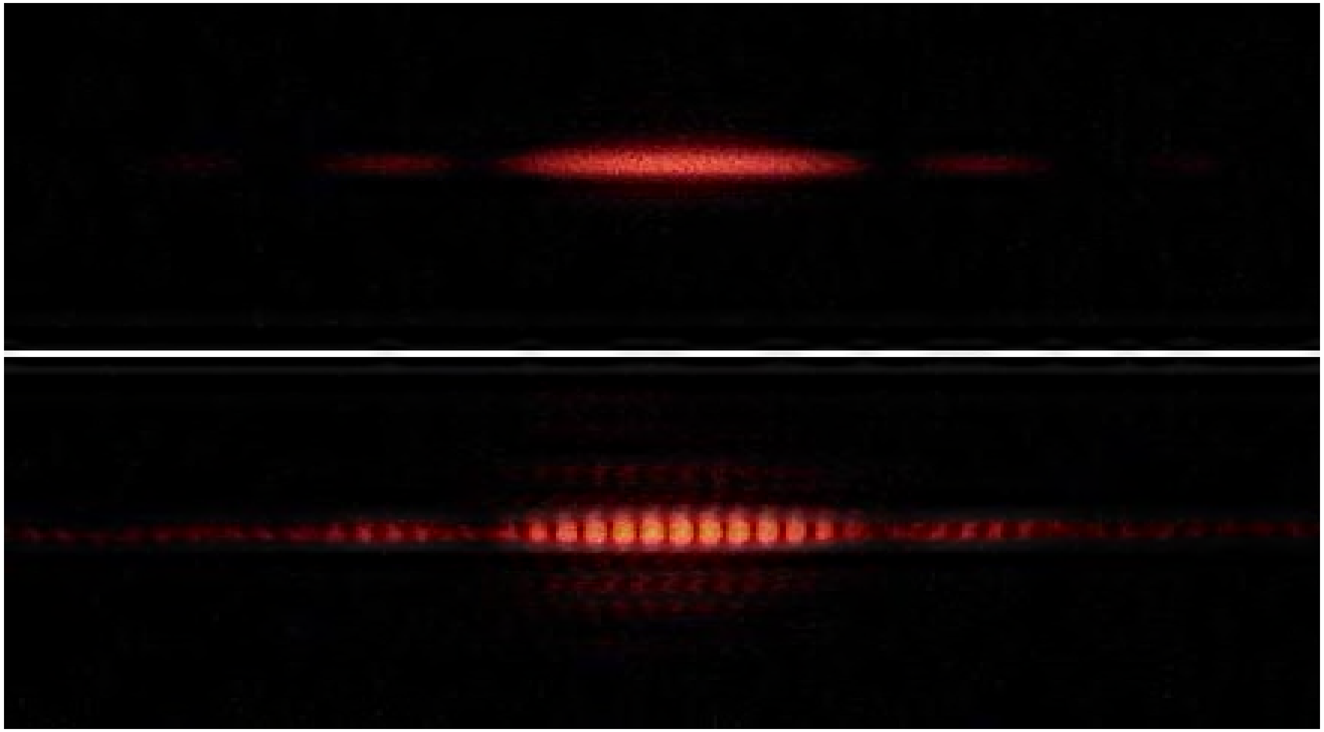
Double-slit pattern. Note the interference fringes, on top of the diffraction pattern.

1. The Double-Slit Experiment

- the following interference pattern shows up: same as before, section in the middle magnified:

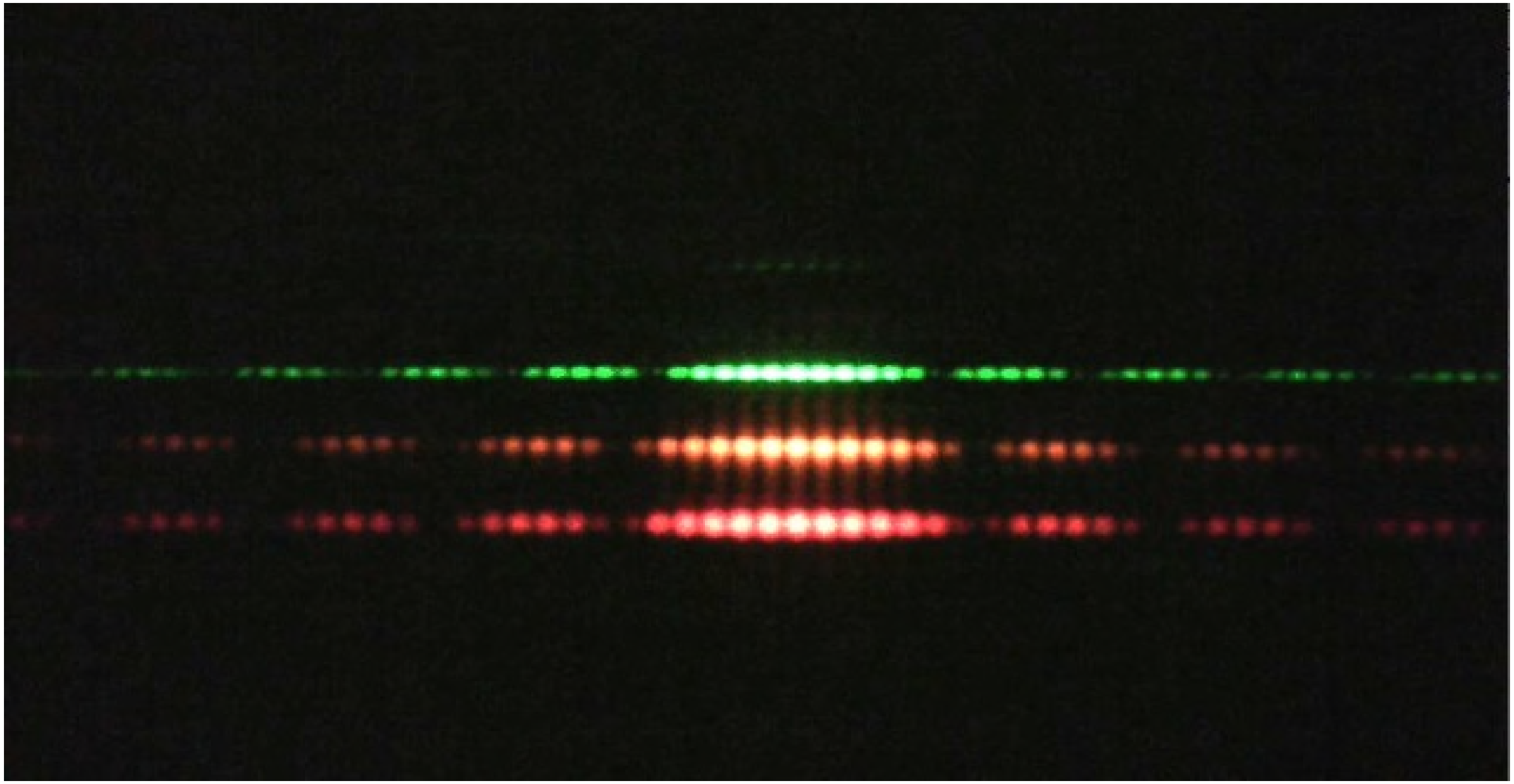
single-slit:

double-slit:



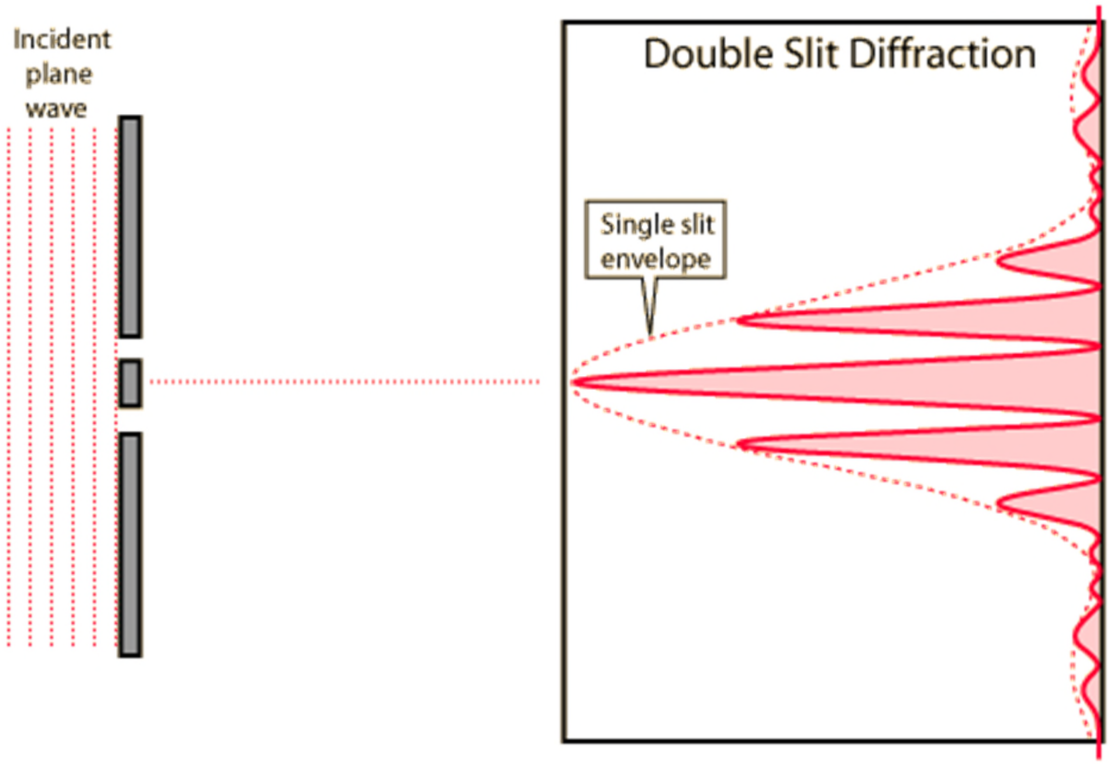
1. The Double-Slit Experiment

- the following interference pattern shows up:
  double-slit, with different wavelengths:



1. The Double-Slit Experiment

- the following interference pattern shows up: single-slit / double-slit :



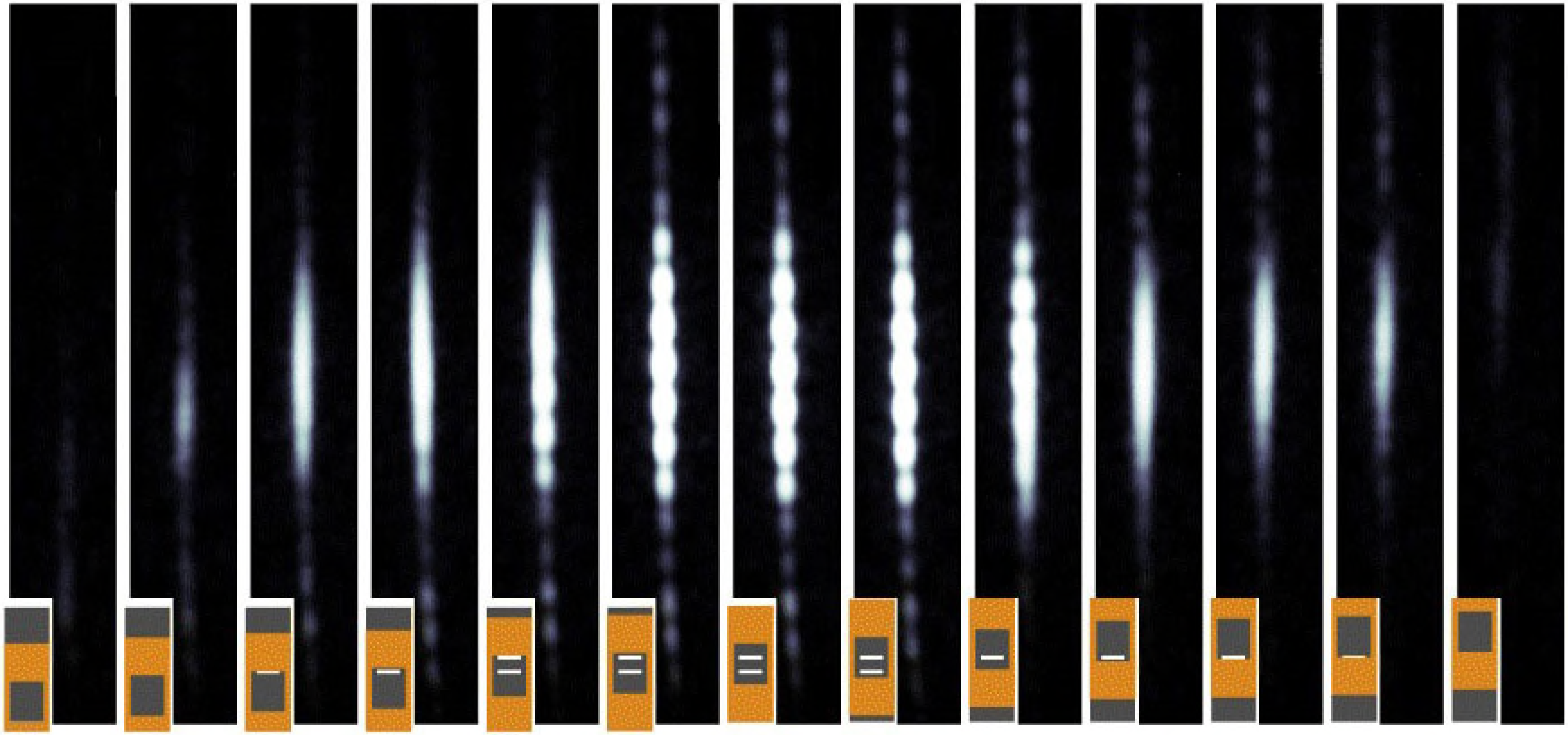
1. The Double-Slit Experiment

- Since these interference pattern are a basic manifestation of the wave-like nature of light: let’s look at the details

$\rightarrow$ calculation on blackboard .

1. The Double-Slit Experiment

- Now, you can do the same thing with electrons:



1. The Double-Slit Experiment

- even if you make sure that at most one electron passes the double-slit at each time, the interference pattern is building up:

  in the following video, there is one electron per second passing through the double-slit:

http://physicsworld.com/cws/article/news/2013/mar/14/feynmans-double-slit-experiment-gets-a-makeover

- The actual experimental setup is quite sophisticated:

  “ The team created a double slit in a gold-coated silicon membrane, in which each slit is 62 nm wide and 4 μm long with a slit separation of 272 nm. To block one slit at a time, a tiny mask controlled by a piezoelectric actuator was slide back and forth across the double slits.”

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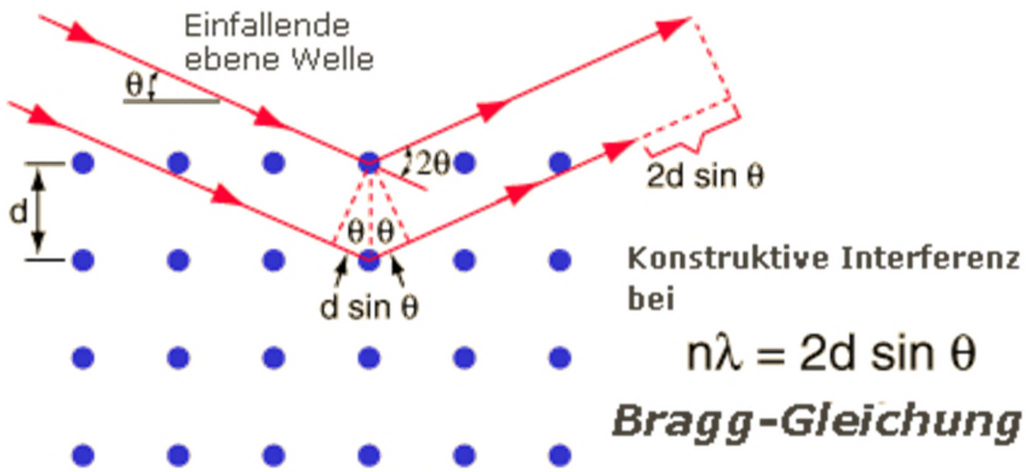
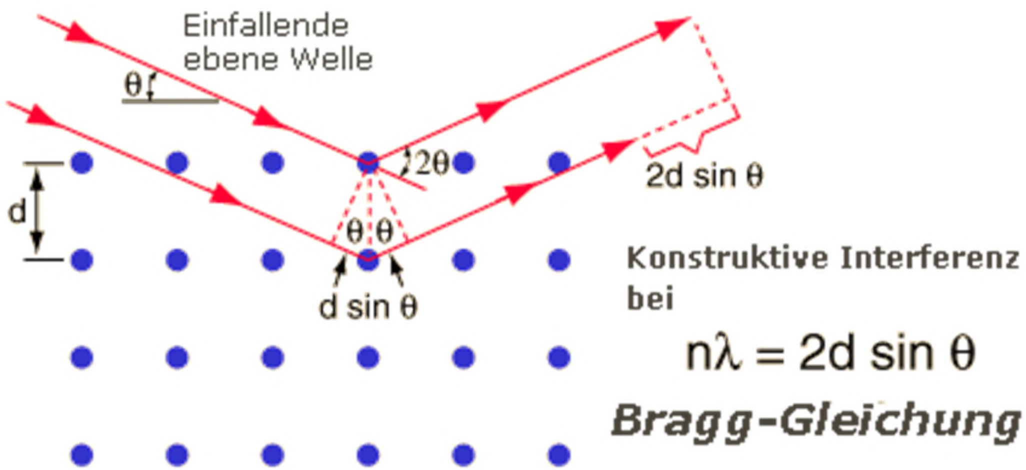
2. Further Interference Experiments

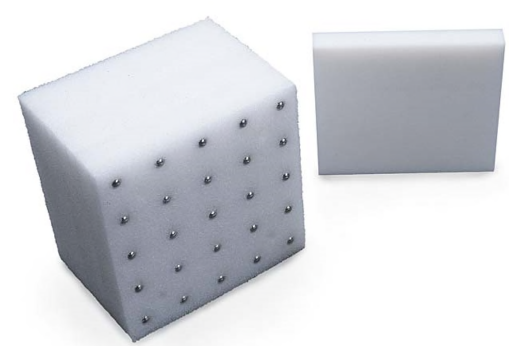
- Historically, the wave-like nature of electrons has not been revealed directly through a double-slit experiment, but through diffraction experiments on crystals whose results looked very similar to those of x-ray (Roentgen-Strahlung) scattering experiments.



2. Further Interference Experiments

- The following experiment can be done with micro waves and the blue dots being aluminum snippets seperated by a centimeter distance (we did that at school..), or with x-rays and the blue dots being atoms in some crystal, or with an electron beam and the blue dots again being atoms in some crystal:



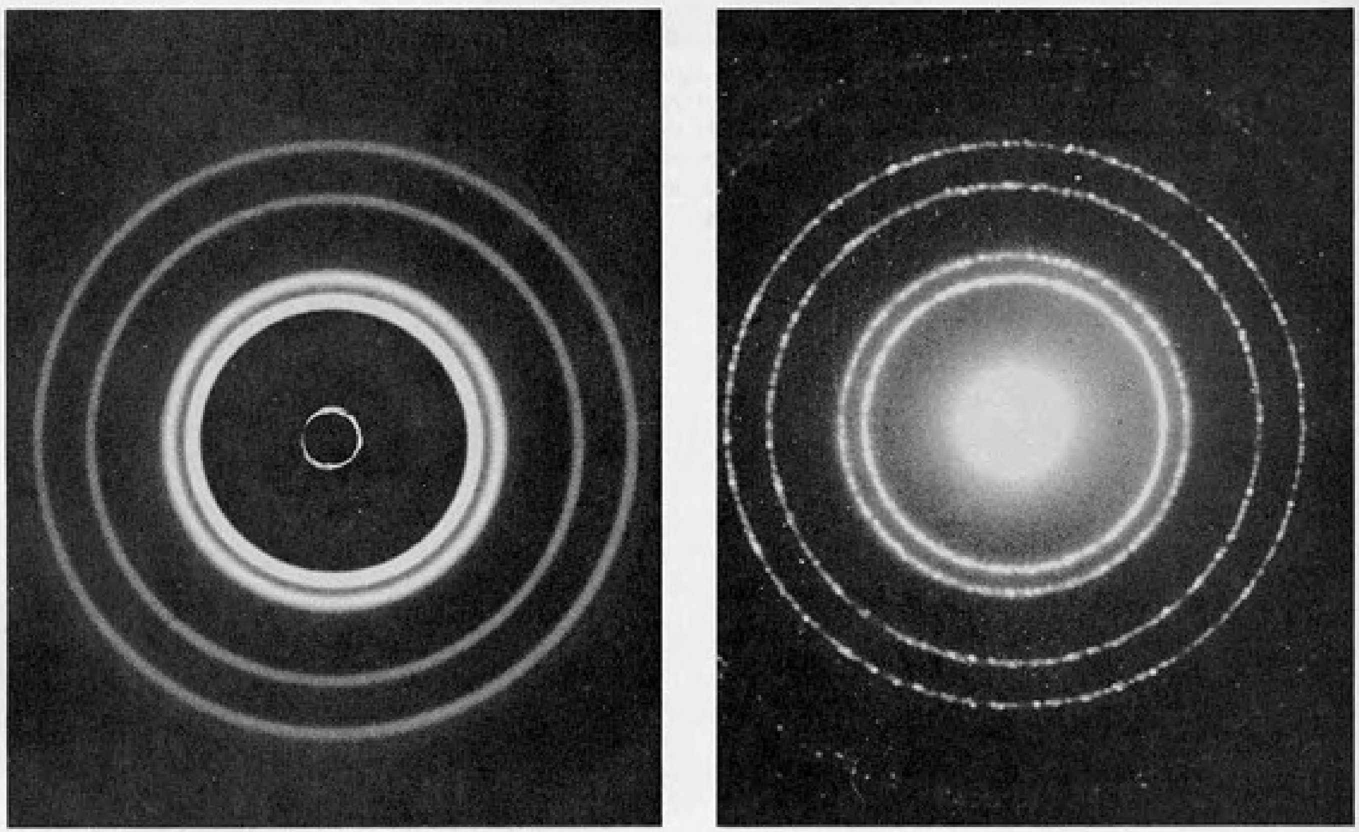


school experiment

2. Further Interference Experiments

- in all cases, a typical interference pattern shows up:

The diffraction pattern on the left was made by a beam of x rays passing through thin aluminum foil. The diffraction pattern on the right was made by a beam of electrons passing through the same foil.



2. Further Interference Experiments

electron diffraction patterns:

monocrystal vs. polycrystal

kaolinite is an industrial mineral
with composition $Al_2Si_2O_5(OH)_4$

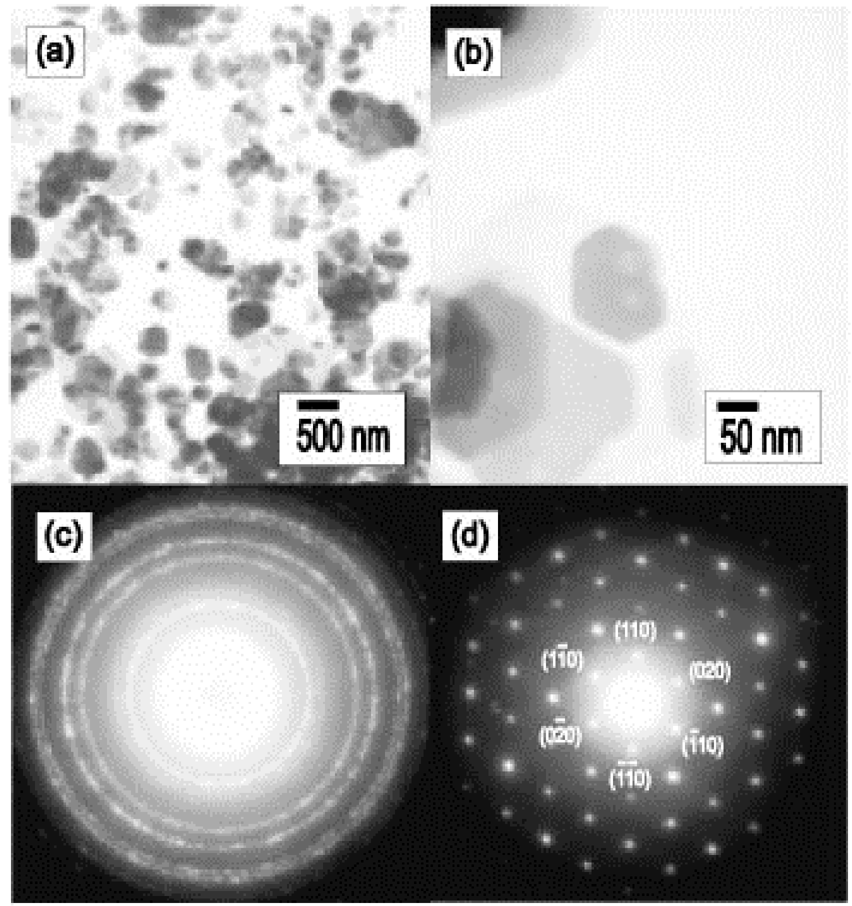
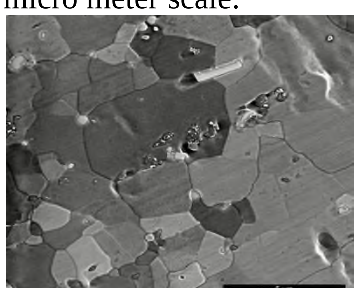


Figure 3. Transmission electron micrographs of PP-0559 kaolinite with magnifications of 15000 x (a) and 150000 x (b). Selected area electron diffraction results are shown in (c) for several kaolinite platelets and in (d) for a single platelet revealing the single crystal nature

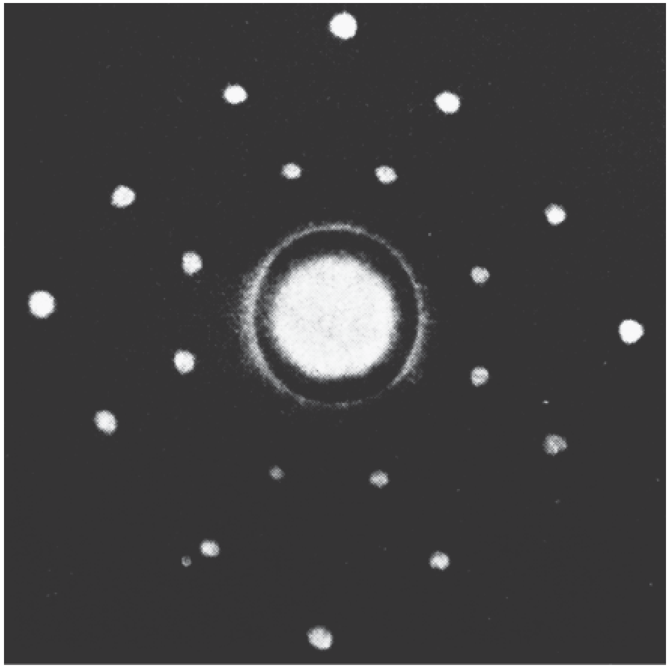
aluminum foil is polycrystalline:

micro meter scale:

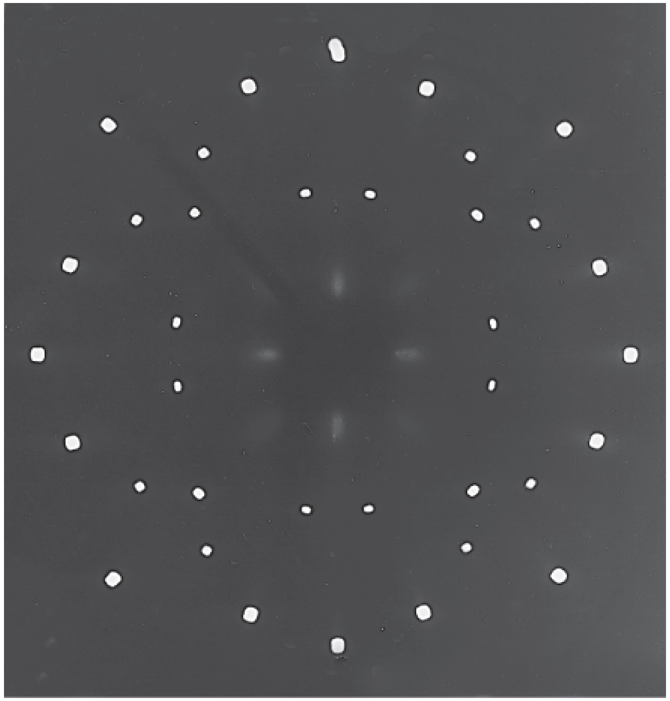


2. Further Interference Experiments

- in all cases, a typical interference pattern shows up:
  diffraction of neutrons (left) vs x-ray diffraction on NaCl crystal:



(*a*)



(*b*)

2. Further Interference Experiments

- diffraction is a standard method in physics and chemistry to analyze materials:

	electron	x-ray	neutron
scattering	by electrostatic repulsion of nucleus	by electron cloud around nucleus	by interaction with the nucleus
resolution	moderate	moderate	high
penetrating power	poor (requires thin specimens)	good	good
matter interaction	high (unreliable results)	none	moderate
magnetic effects	no	no	yes (neutrons have their own magnetic field)
good for light elements	no	no	yes
particular uses	crystals	crystals	fuel rods, archaeological artefacts

(scattering/electron should read: electrostatic interaction with nucleus and electrons)

2. Further Interference Experiments

- DNA has been decoded by x-ray diffraction:

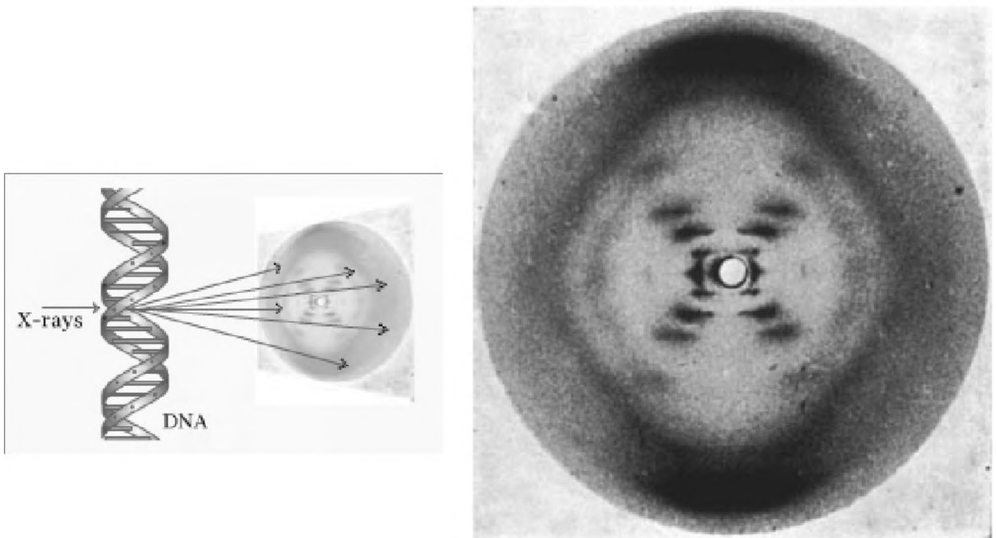


FIGURE 2.18. The crucial X-ray diffraction image of the B form of DNA (Photograph 51) taken by Rosalind Franklin and Ray Gosling. The X-shaped pattern in this image meant that the DNA molecule was a helix, critical information for Watson and Crick's model building.

2.18, courtesy of the James D. Watson Collection, CSHL Library and Archives

Rosalind Franklin

2. Further Interference Experiments

Laser light analog
of Rosalind Franklin's
"Photograph 51" :

(at a 2010 meeting of
the American Physical
Society)

How Rosalind Franklin Discovered the Helical Structure of DNA

March Meeting 2010

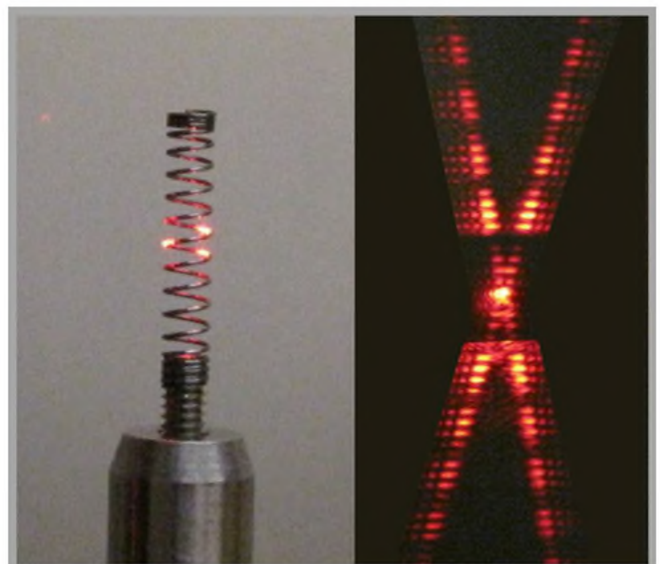
When illuminated with a laser pointer, a spring of a ballpoint pen produces a diffraction pattern which is similar to the famous Photo 51 of helical DNA

Heidrun Schmitzer
Dennis Tierney
Gregory Braun
Xavier University
Department of Physics
Cincinnati, Ohio

Abstract

K1.00020: "How Rosalind Franklin Discovered the Helical Structure of DNA: Experiments in diffraction"

Presented Tuesday, March 16, 2010



The left photo shows the illuminated spring. The right photo is the diffraction pattern produced by the spring, when five turns are illuminated. It was taken at a distance of ~12m behind the spring. The pattern shows the same structure as Rosalind Franklin's X-ray diffraction image of helical DNA.

The angle of the upper and lower conical section are equivalent to the double pitch angle of the helix. The structure in the areas with maxima is caused by the multiple pitch diffraction and reveals the diameter of the helix. Note that the center of the right pattern was covered with a polarizer set almost to extinction to avoid over exposure at the very bright center maximum. Franklin used a lead disc for the same purpose in the X-ray photo.

2. Further Interference Experiments

- Meanwhile interference has been demonstrated with quite large molecules:

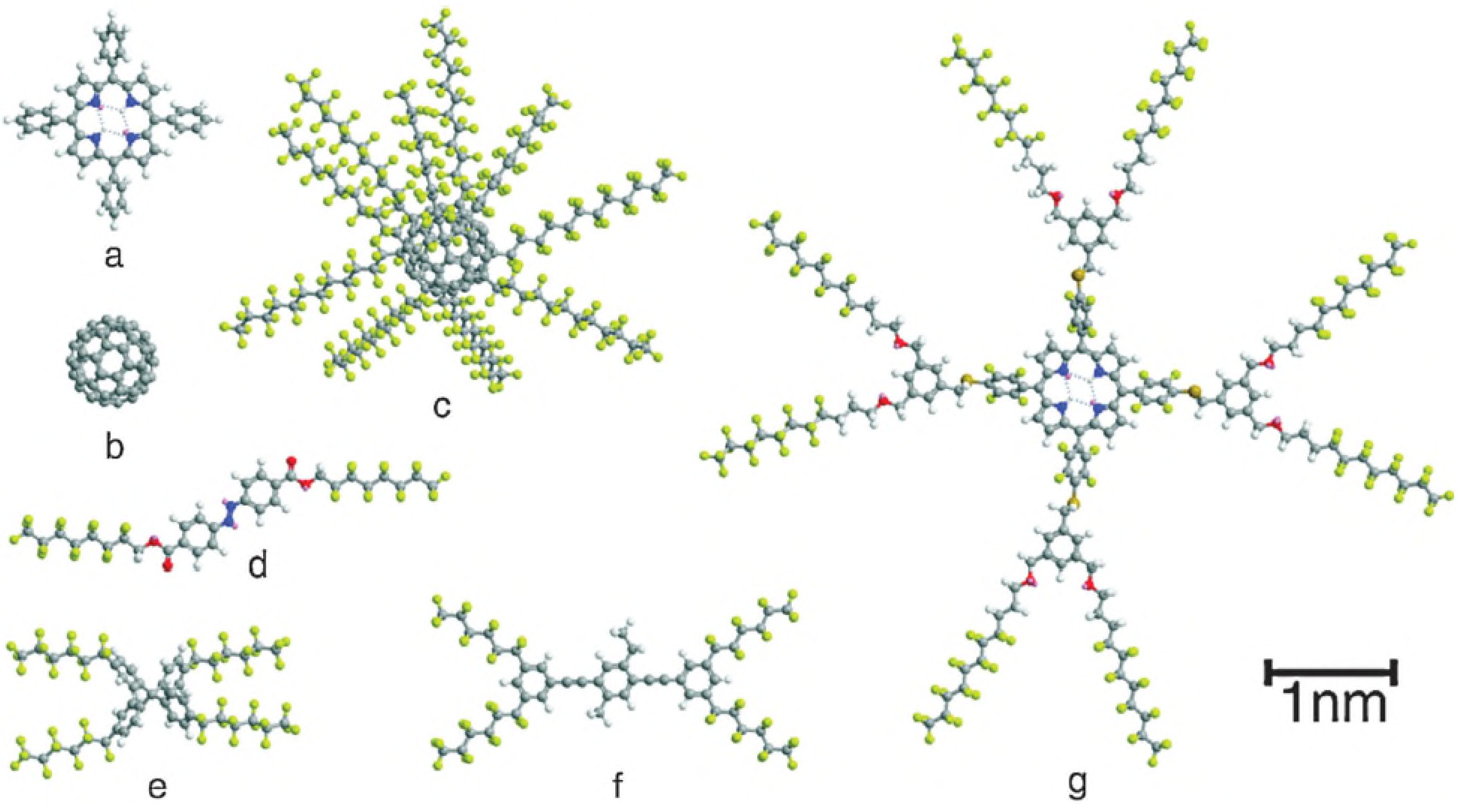


FIG. 7 (color). Gallery of molecules that showed quantum interference in the KDTL interferometer. (a) Tetraphenylporphyrin (TPP); (b) C_{60} fullerene; (c) PFNS10, a carbon nanosphere with ten perfluroalkyl chains; the variant PFNS8 with eight side arms was also used; (d) a perfluoroalkyl-functionalized diazobenzene (Gerlich *et al.*, 2007); (e), (f) two structural isomers with equal chemical composition but different atomic arrangement (Tüxen *et al.*, 2010); (g) TPPF152, a TPP derivative with 152 fluorine atoms (Gerlich *et al.*, 2011).

Content:

Part I :

Part II :

3. The Postulates of Quantum Mechanics

- The postulates of quantum mechanics connect things from the real world with things in a physical theory formalized by mathematical expressions and equations.
- Since the real world is not a mathematical object, the postulates of quantum mechanics cannot be compared to, for example, the axioms of the real numbers which is something which takes place purely in a mathematics-world.
- For example, in our second talk we want to calculate the energy spectrum of the hydrogen atom. Since the hydrogen atom has only one electron, we don’t have to say anything about the modelling of multi-particle states, we don’t have to say anything about fermions and bosons. We also can ignore electron spin since we won’t apply any magnetic fields.

3. The Postulates of Quantum Mechanics

- As a result, depending on where you look, which book or which web-page, you can find lists with postulates ranging from 2 or 3 up to 8 or 9 postulates.

- For our purposes, the following list with 4 postulates is appropriate:

  (P1) Quantum state $\rightarrow$ a normalized vector in a Hilbert space
  (P2) Observable $\rightarrow$ Hermitian operator
  (P3) Possible measurement values of observable M $\rightarrow$ eigenvalues of $\hat{M}$
  (P4) Time-evolution of a quantum state $\rightarrow$ Schroedinger equation

- In more detail:

3. The Postulates of Quantum Mechanics

- Postulates (P1) and (P2):

Postulate	Classical Mechanics	Quantum Mechanics
I	A state of a classical system is given by a pair $(x(t), p(t)) \in \mathbb{R}^6$ with $x(t)$ being the position and $p(t)$ being the momentum of the particle at time t.	A state of the quantum system is given by a vector $\psi(t)$ in some Hilbert space $\mathcal{H}$. In coordinate space representation, $\mathcal{H} = L^2(\mathbb{R}^3)$ and $\lvert\psi(x,t)\rvert^2 d^3x$ is the probability of finding the particle at x in the volume element d^3x at time t.
II	A physical measurable quantity M is given by a real valued function $M(x, p)$ of position x and momentum p.	Let the position operator $\hat{x}$ and the momentum operator $\hat{p}$ be given by $\hat{x}\psi = x\psi(x,t)$, multiplication with x, and $\hat{p}\psi = \frac{\hbar}{i}\nabla\psi$. Then the measurable quantity M is represented by a self-adjoint operator $\hat{M} = M(\hat{x}, \hat{p})$.

3. The Postulates of Quantum Mechanics

- Postulate (P2): M and $\hat{\mathrm{M}}$ for the most important observables:

Physikalische Grösse	klassisch	Operator
Ortsvektor	$\vec{r} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$	$\hat{\vec{r}} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$
Impulsvektor	$\vec{p} = \begin{pmatrix} p_x \\ p_y \\ p_z \end{pmatrix}$	$\hat{\vec{p}} = \frac{\hbar}{i} \begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{pmatrix}$
Hamilton-Funktion	$H = E = \frac{p^2}{2m} + V(x, y, z)$	$\hat{H} = -\frac{\hbar^2}{2m}\Delta + V(x, y, z)$
Bahndrehimpulsvektor	$\vec{L} = \begin{pmatrix} yp_z - zp_y \\ zp_x - xp_z \\ xp_y - yp_x \end{pmatrix}$	$\hat{\vec{L}} = \frac{\hbar}{i} \begin{pmatrix} y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y} \\ z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z} \\ x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x} \end{pmatrix}$

3. The Postulates of Quantum Mechanics

- Postulates (P3) and (P4):

Postulate	Classical Mechanics	Quantum Mechanics
III	A measurement of M is $M(x,p)$. The act of measurement does not disturb the state of the system.	A measurement of M yields a value from the set of eigenvalues of $\hat{M}$. If ψ_n is a normalized eigenvector of $\hat{M}$ with eigenvalue λ_n, then the probability of obtaining λ_n as a result of the measurement on the system in the normalized state ψ is given by $\lvert\langle\psi,\psi_n\rangle\rvert^2$. As a result of the measurement process, the state of the system suddenly changes from ψ to ψ_n.
IV	The time evolution of the state is given by Newton's equation $$\begin{aligned} \frac{d}{dt}x(t) &= \frac{p(t)}{m} \\ \frac{d}{dt}p(t) &= F\big(x(t),p(t),t\big) \end{aligned}$$	The time evolution of the state of the system is given by the time dependent Schrödinger equation $$i\hbar\frac{d}{dt}\psi(t) = \hat{H}\psi(t)$$ where $\hat{H}$ is the operator corresponding to the classical Hamiltonian, kinetic plus potential energy, of the system.

3. The Postulates of Quantum Mechanics

- In postulate (P3) it is stated:
  "As the result of the measurement process, the state of the system suddenly changes from psi to psi_n"

- This is formulated as a postulate since actually one does not really know of what exactly is going on.

- The process itself is referred to as "wave-function collapse". So this is something at the very bottom of quantum mechanics.

3. The Postulates of Quantum Mechanics

- In the last 15-20 years there has been considerable research activity on this issue. A very nice, very readable and quite recent overview over the subject has been given in "Models of Wave-function Collapse, Underlying Theories, and Experimental Tests" by Angelo Bassi, Kinjalk Lochan, Seema Satin, Tejinder P. Singh and Hendrik Ulbricht:

  https://arxiv.org/abs/1204.4325

- In section 5 we demonstrate a (or, "the"?) mechanism for wave-function collapse in a simple demo-model.

Content:

Part I :

Part II :

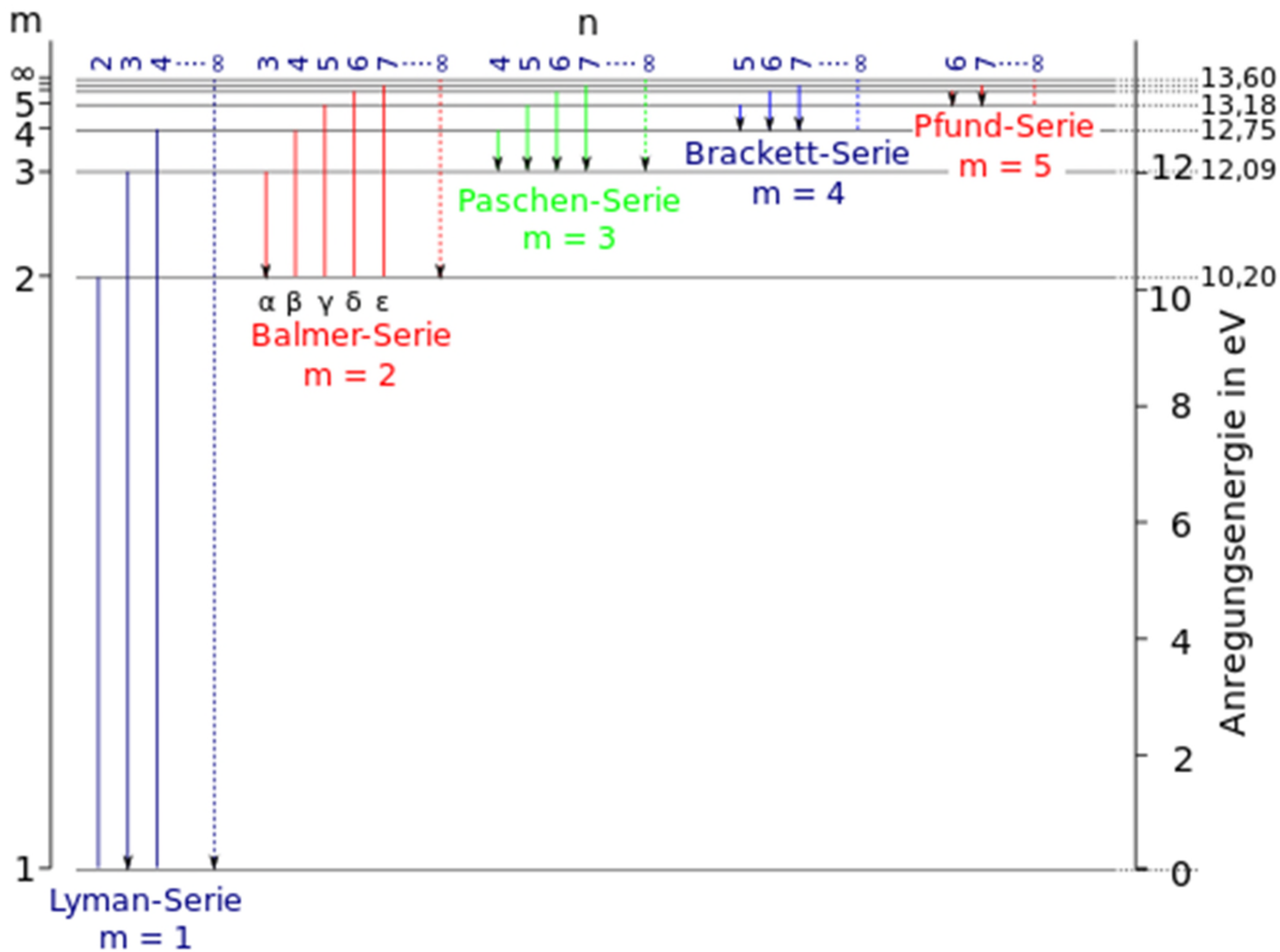
4. The Energy Spectrum of the Hydrogen Atom

..we do this on the blackboard.

- The Balmer series is in the visible spectrum of the H-atom:

4. The Energy Spectrum of the Hydrogen Atom

- energy levels in the H-atom:



4. Appendix to Radial Eigenfunctions:

- There is the following result: (from Szego: Orthogonal Polynomials, 1939)

5.7. Closure

Here we prove the analogue of Theorem 3.1.5 for Laguerre and Hermite polynomials. The main difficulty of these cases is due to the fact that the orthogonality interval is infinite. Using the customary notation (§1.1), we have the following theorem:

THEOREM 5.7.1. *The system*

$$e^{-x/2}x^{\alpha/2}x^n, \qquad \alpha > -1,\ n = 0, 1, 2, \cdots, \tag{5.7.1}$$

is closed in $L^2(0, +\infty)$; *the system*

$$e^{-x^2/2}x^n, \qquad n = 0, 1, 2, \cdots, \tag{5.7.2}$$

is closed in $L^2(-\infty, +\infty)$.

This statement is equivalent to the closure of the systems $\{e^{-x/2}x^{\alpha/2}L_n^{(\alpha)}(x)\}$ and $\{e^{-x^2/2}H_n(x)\}$, respectively. Theorem 5.7.1 remains true, of course, if we replace $e^{-x/2}$ by e^{-x} and $e^{-x^2/2}$ by e^{-x^2}, respectively. The idea of the following proof is due to J. von Neumann (see Hilbert-Courant **1**, pp. 81–82).

4. Appendix to Radial Eigenfunctions:

- The first statement (5.7.1) means that (taking alpha=4 and alpha=10)

$$x^2 , x^3 , x^4 , x^5 , x^6 , x^7 \ldots \qquad \text{times} \ \exp(-x/2)$$

is a basis of $L^2(0,\infty)$, but that

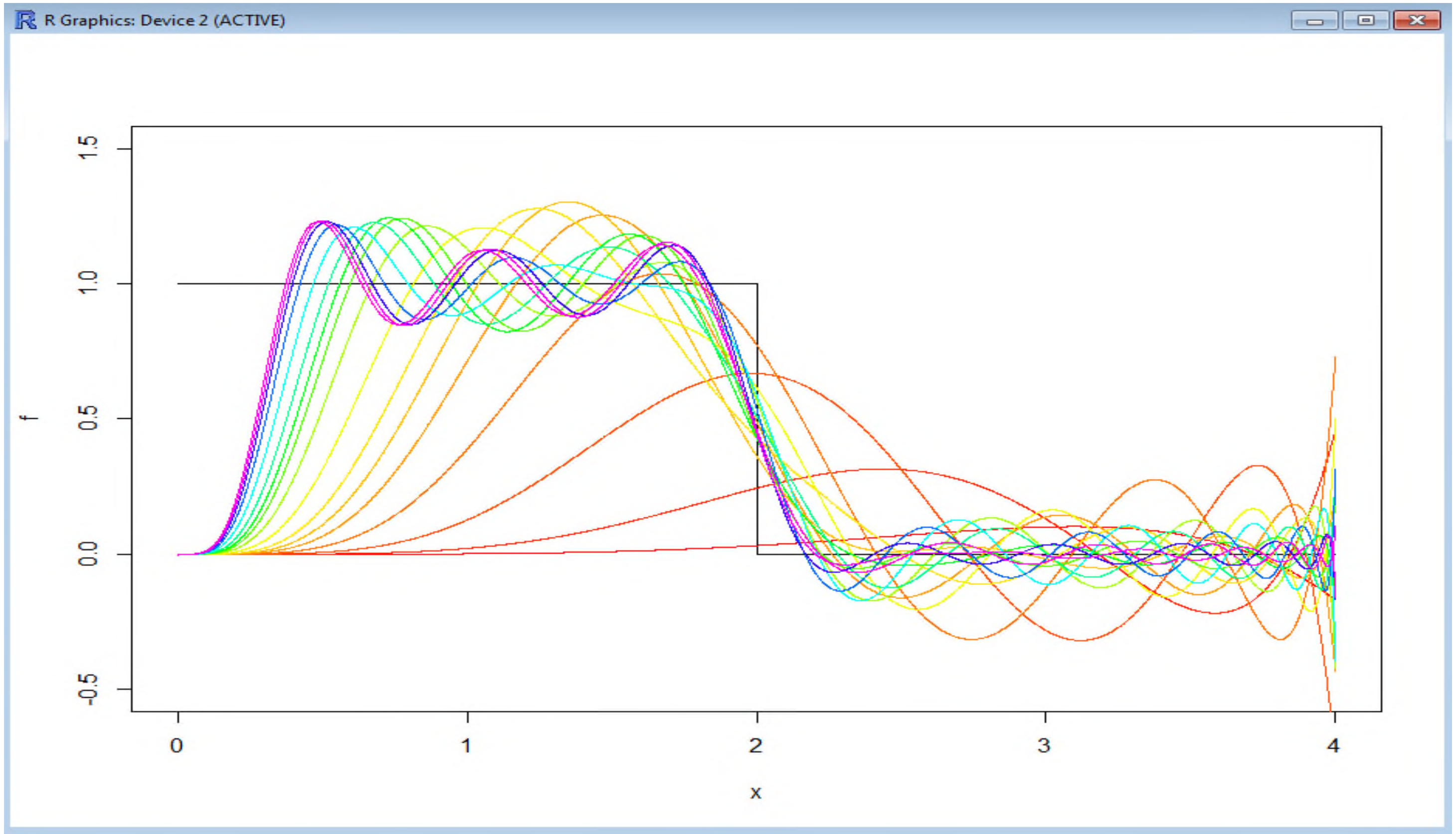
$$x^5 , x^6 , x^7 \ldots \qquad \text{times} \ \exp(-x/2)$$

is also a basis of $L^2(0,\infty)$.

Since this looks somewhat counter intuitive, let’s make a quick R-simulation:

4. Appendix to Radial Eigenfunctions:

- expanding a step function chi_[0,2](x) on [0,4] with respect to the polynomials x^5, x^6, x^7, ... , x^40   (starting with x^15 there are numerical issues..)



4. Appendix to Radial Eigenfunctions:

- "the system is closed" in the book of Szego means actually complete:

1.5. Closure; integral approximations

(1) DEFINITION. *Let* $p \geqq 1$, *and let* $\alpha(x)$ *be a non-decreasing function in* $[a, b]$ *which is not constant.*[4] *Let the functions*

$$f_0(x), f_1(x), f_2(x), \cdots, f_n(x), \cdots \tag{1.5.1}$$

be of the class $L_\alpha^p(a, b)$. *The system* (1.5.1) *is called closed in* $L_\alpha^p(a, b)$ *if for every* $f(x)$ *of* $L_\alpha^p(a, b)$ *and for every* $\epsilon > 0$ *a function of the form*

$$k(x) = c_0 f_0(x) + c_1 f_1(x) + \cdots + c_n f_n(x) \tag{1.5.2}$$

exists such that

$$\int_a^b |f(x) - k(x)|^p \, d\alpha(x) < \epsilon. \tag{1.5.3}$$

With regard to this definition see Kaczmarz-Steinhaus **1**, p. 49. These authors use the term "Abgeschlossenheit" for "closure."

Content:

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5. A Closer Look at the Postulates: Wave-Collapse Models

- Quick reminder: In postulate (P3) it is stated:
  "As the result of the measurement process, the state of the system suddenly changes from psi to psi_n"

- This is formulated as a postulate since actually one does not really know of what is going on there.

- The process itself is referred to as "wave-function collapse". So this is something at the very bottom of quantum mechanics.

5. A Closer Look at the Postulates: Wave-Collapse Models

- The Schroedinger equation is a linear equation:
  If psi_1 and psi_2 are two solutions, then also the sum is a solution.
- This is not just taken as a mathematical fact, but has the following physical interpretation:
  If psi_1 is a solution which corresponds to physical reality, for example, the electron is at position P1 in space, and if psi_2 is a solution which corresponds to physical reality, for example, the electron is at position P2 in space, then the wavefunction

$$psi := 1/sqrt(2) * psi_1 + 1/sqrt(2) * psi_2$$

is not just mathematically a solution of the Schroedinger equation, but the interpretation is, that this actually corresponds to a physical reality.

5. A Closer Look at the Postulates: Wave-Collapse Models

- Apparently, makroscopic objects have unique positions in space.
- So you can't just say, I take a football and two wave functions which locate the football at positions P1 and P2 respectively and then the combined wave function

  $$\text{psi} := 1/\text{sqrt}(2) * \text{psi}_1 + 1/\text{sqrt}(2) * \text{psi}_2$$

  locates the football simultaneously at positions P1 and P2.
- In other words, the superposition principle does not hold for makroscopic objects.
- Now, the overwhealming majority of physicists (and I would think also the people in this room) share the deep believe that there must be some universal theory of nature which applies to all scales, not just one theory for microscopic things and another theory for makroscopic issues. At least, in principle.

5. A Closer Look at the Postulates: Wave-Collapse Models

- Wave-collapse models are an attempt to interpolate between quantum mechanics and classical mechanics with a unified theory, which has both quantum mechanics and classical mechanics as limiting cases.

The basic mathematical mechanism which should do this is as follows:

(see the notes "Wave-function Collapse Models: The Basic Mechanism" on the summer school web page)

5. A Closer Look at the Postulates: Wave-Collapse Models

- Let's simulate the SDE-system (12), (8):
- We take an N-state system with energies

$$\mathrm{eps}_n = n \qquad \text{for} \quad n = 1, 2, \ldots, N$$

- The initial state is a superposition of eigenstates with equal probability for each eigenstate. That is,

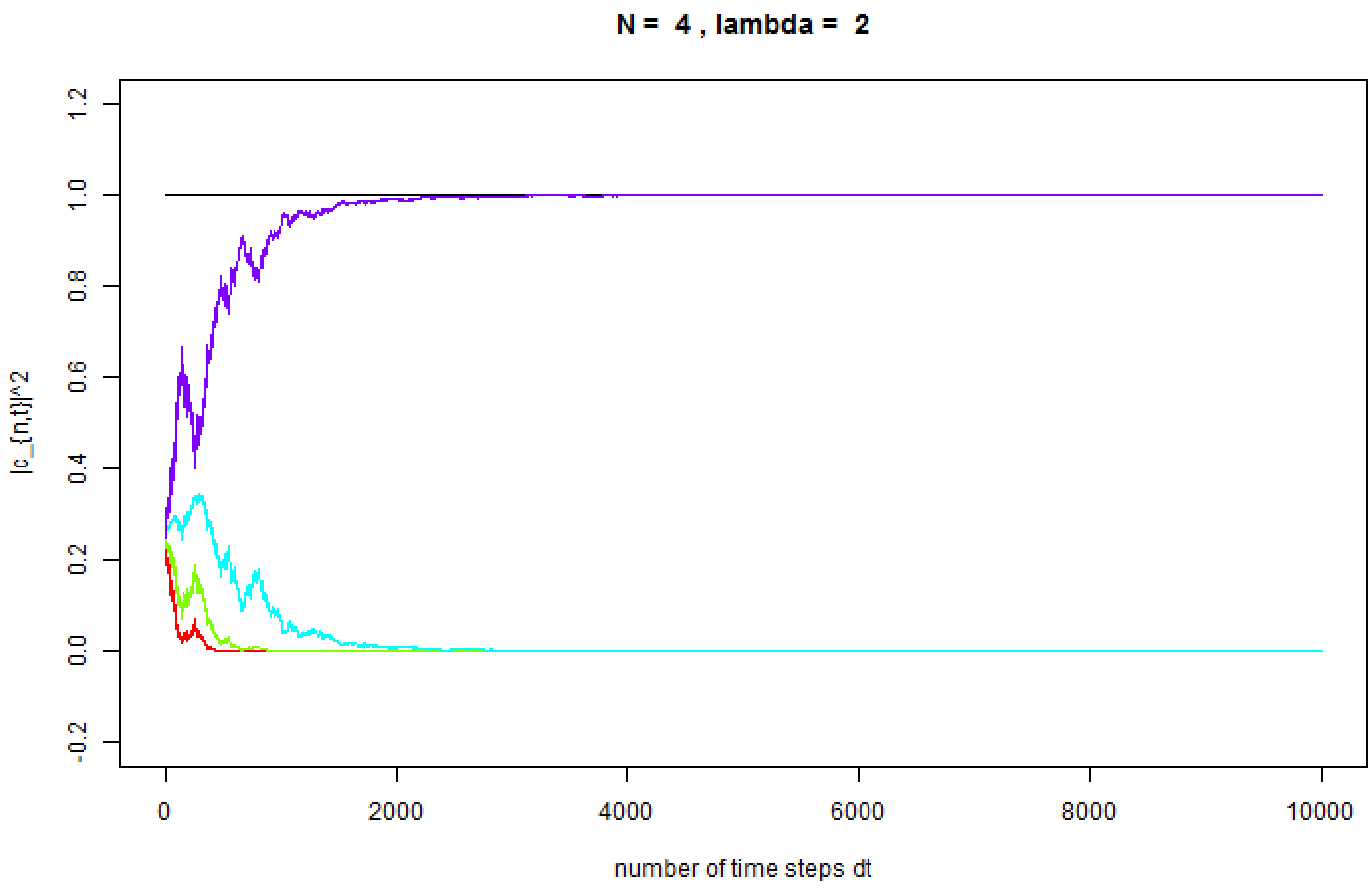
$$|c_{n,0}|^2 = 1 / N \qquad \text{for} \quad n = 1, 2, \ldots, N$$

- We would like to see that, as time evolves, exactly one of the $|c_{n,t}|$ converges to 1, and all the other $c_{n,t}$ converge to zero, depending on which Brownian path has realized:

“the wave function has collapsed onto the eigenstate phi_n”

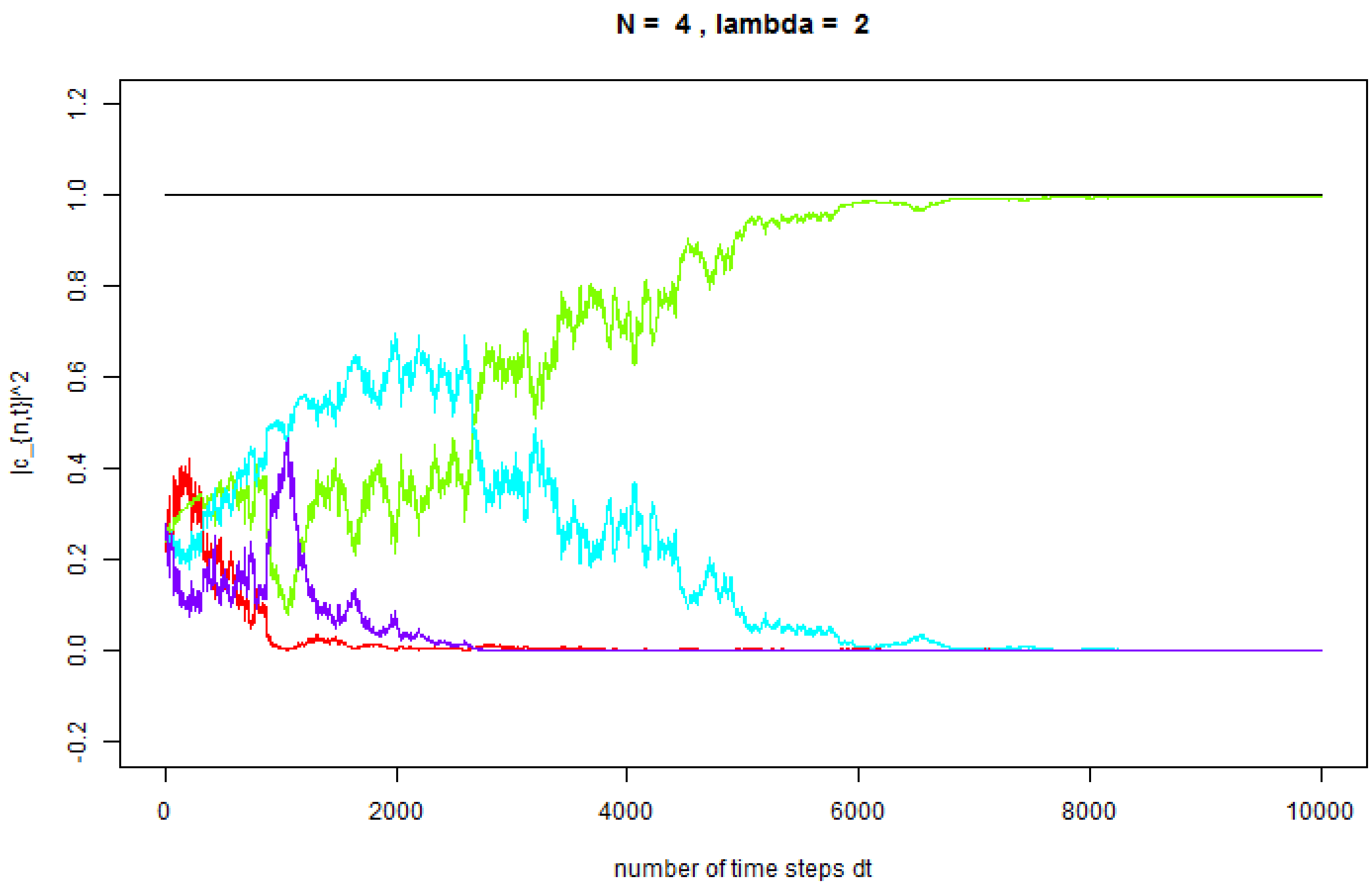
5. A Closer Look at the Postulates: Wave-Collapse Models

- Exactly this behaviour can be seen: T = 1, N = 4, lambda = 2:



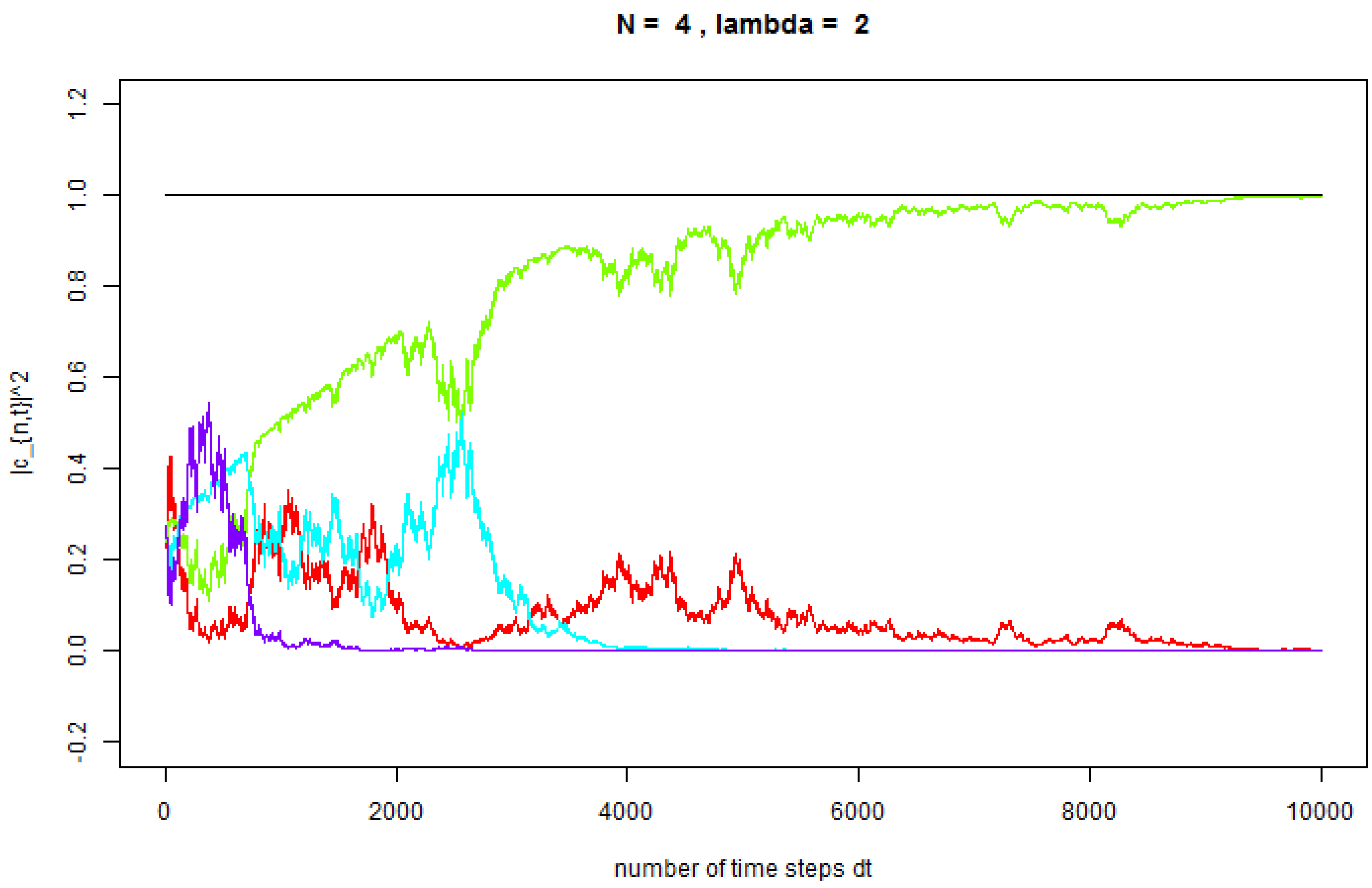
5. A Closer Look at the Postulates: Wave-Collapse Models

- Exactly this behaviour can be seen: different random numbers



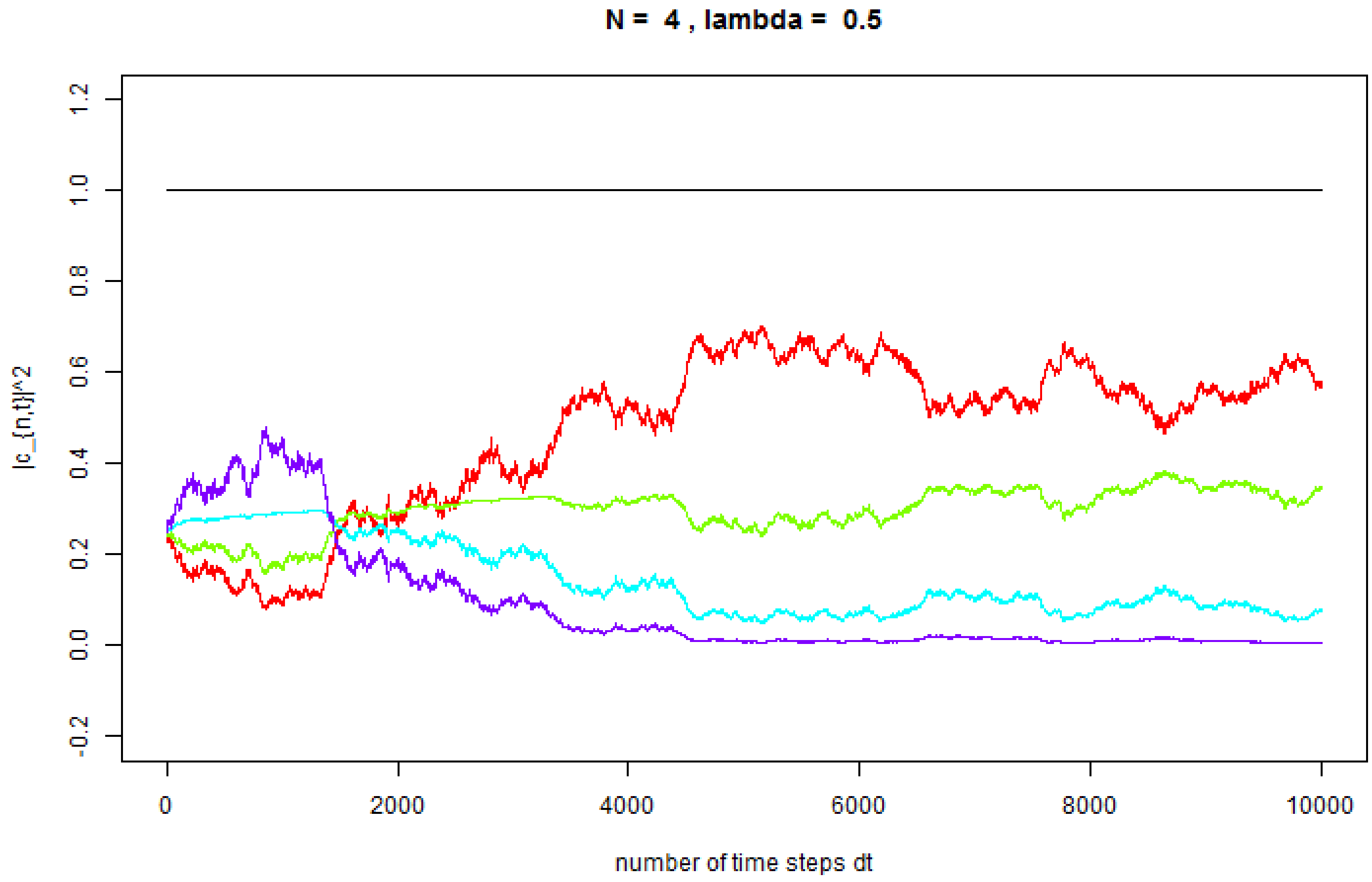
5. A Closer Look at the Postulates: Wave-Collapse Models

- Exactly this behaviour can be seen: different random numbers



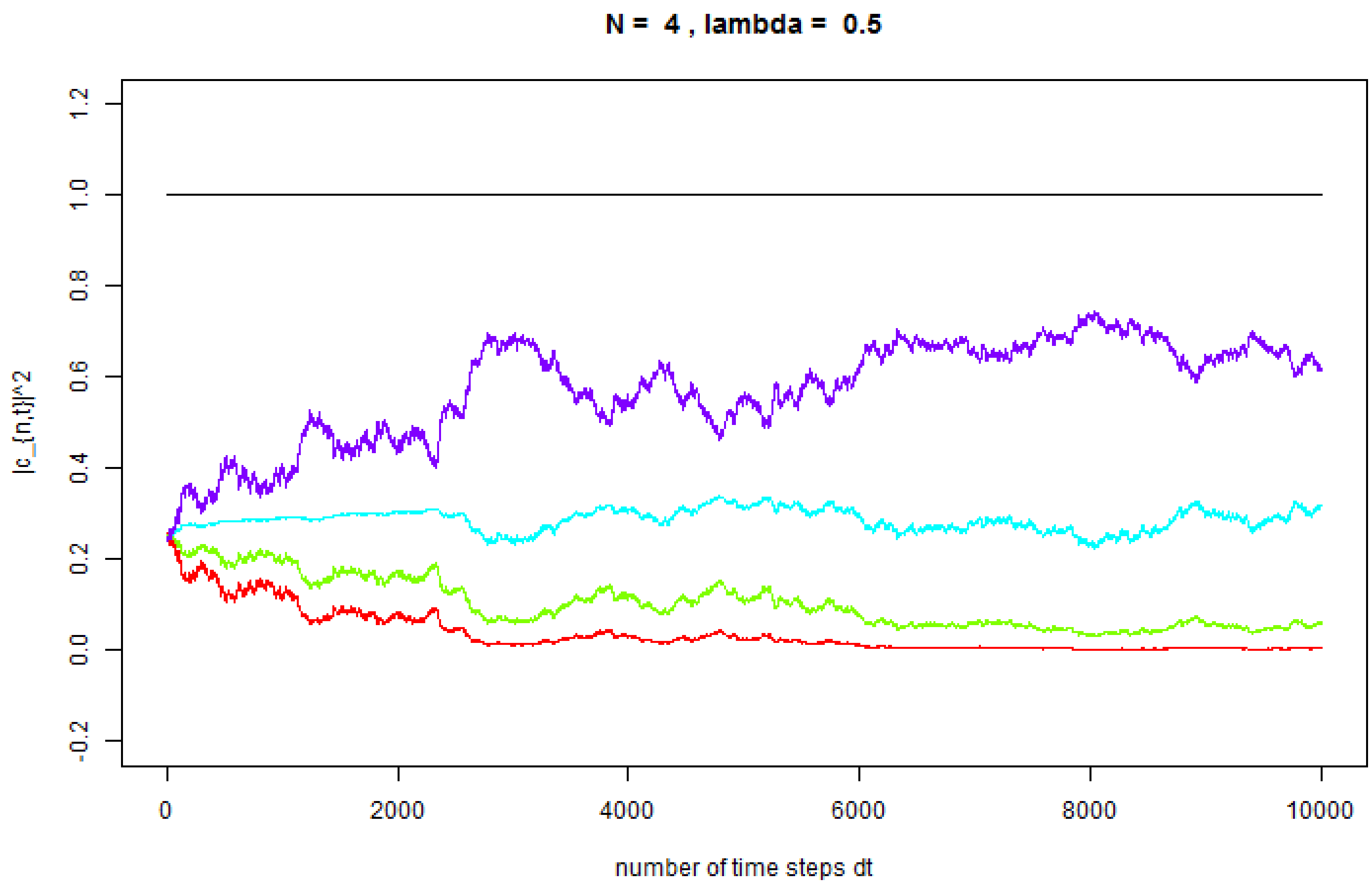
5. A Closer Look at the Postulates: Wave-Collapse Models

- N = 4, now lambda smaller: lambda = 0.5



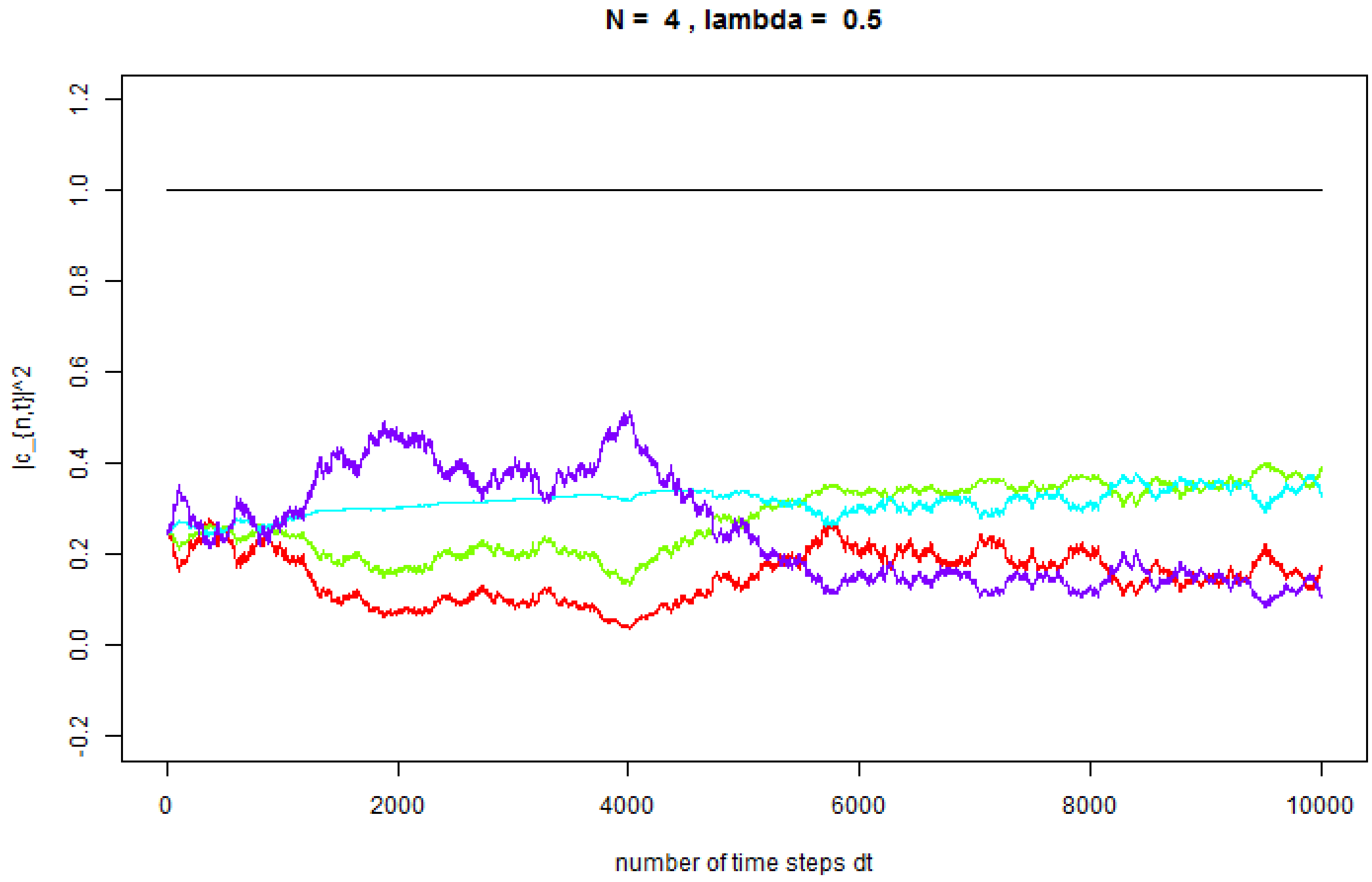
5. A Closer Look at the Postulates: Wave-Collapse Models

- N = 4, now lambda smaller: lambda = 0.5, different random numbers



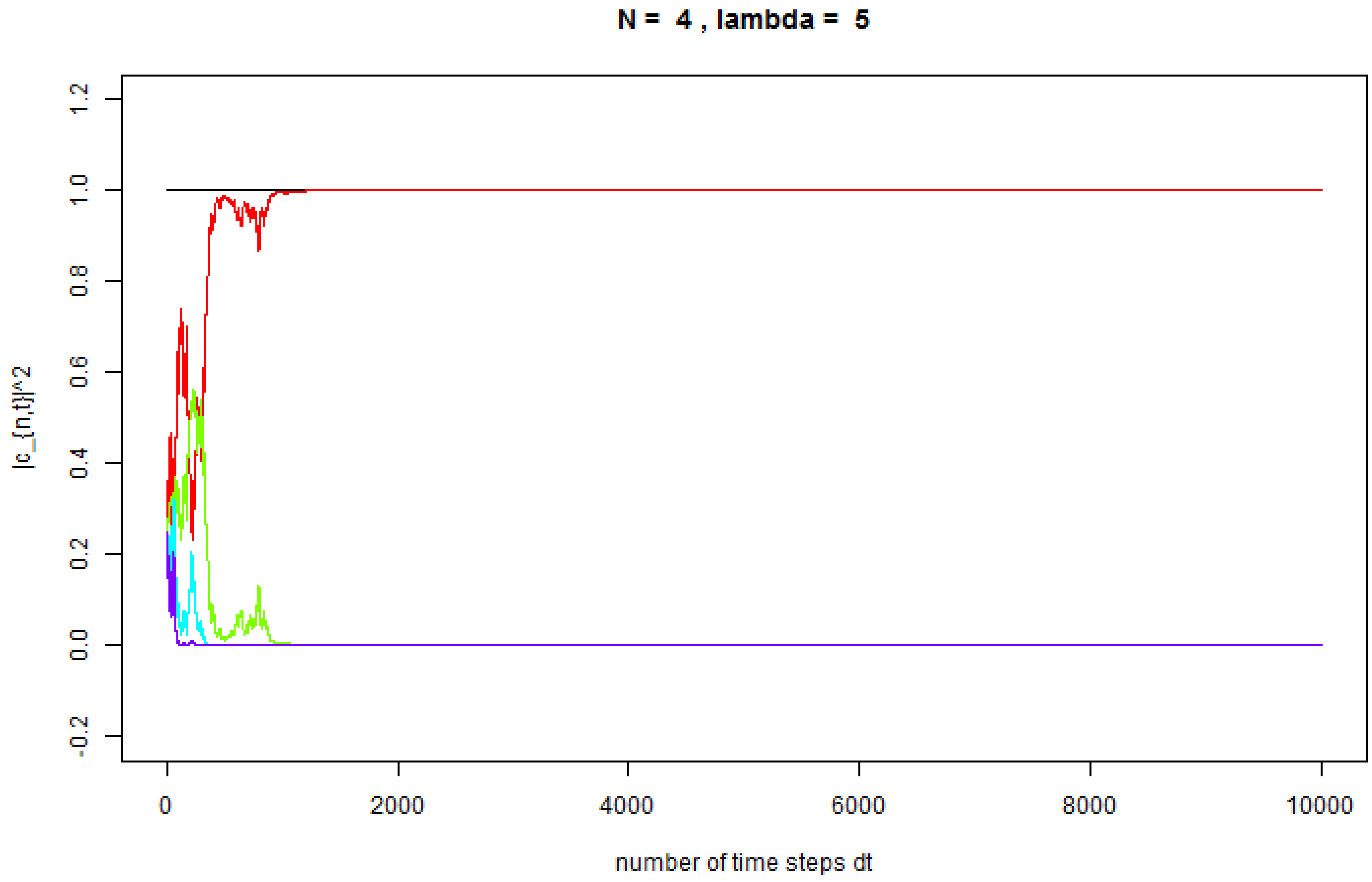
5. A Closer Look at the Postulates: Wave-Collapse Models

- N = 4, now lambda smaller: lambda = 0.5, different random numbers



5. A Closer Look at the Postulates: Wave-Collapse Models

- N = 4, now lambda larger: lambda = 5



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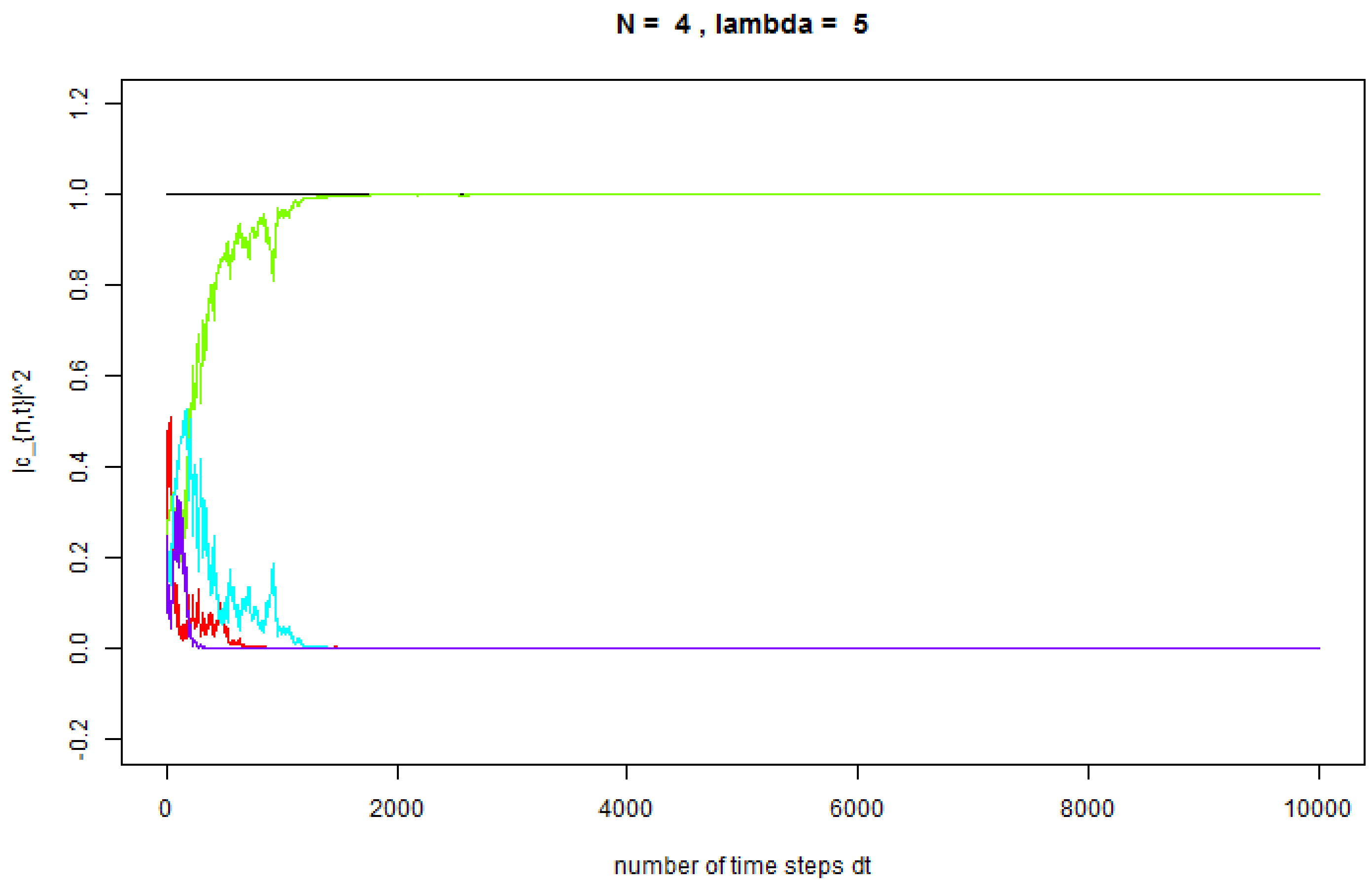
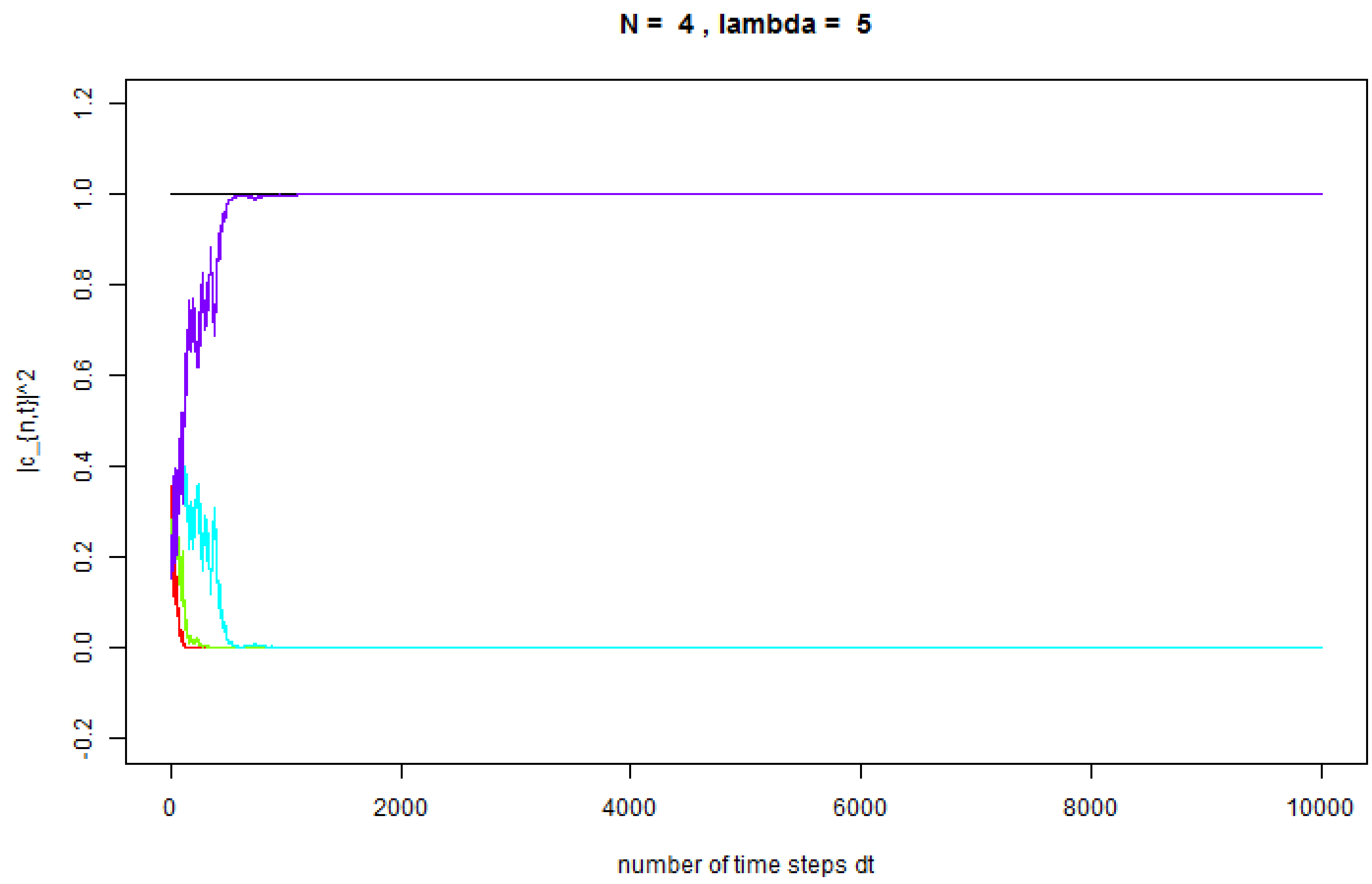
- N = 4, now lambda larger: lambda = 5, different random numbers



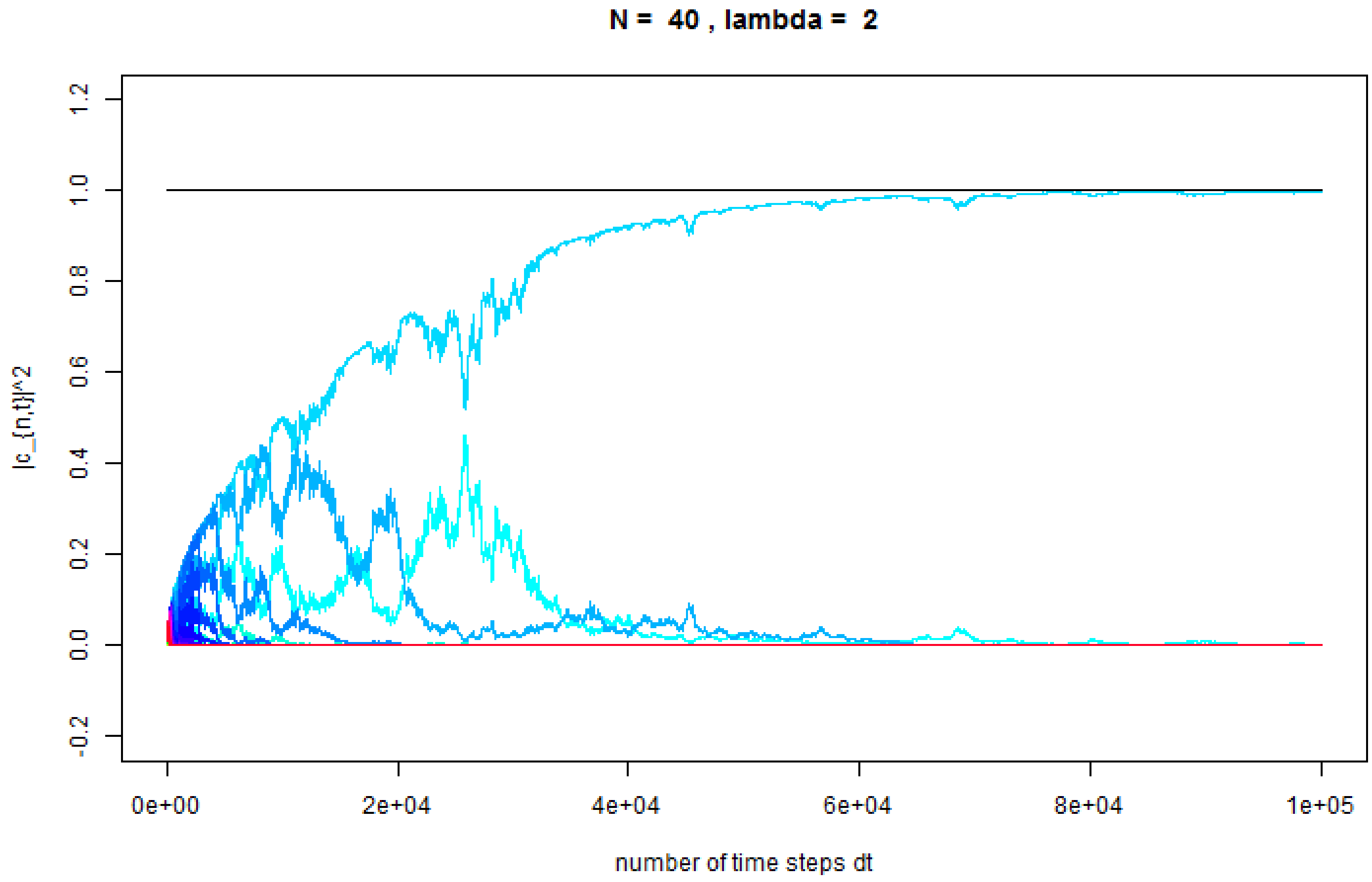
5. A Closer Look at the Postulates: Wave-Collapse Models

- N = 4, now lambda larger: lambda = 5, different random numbers



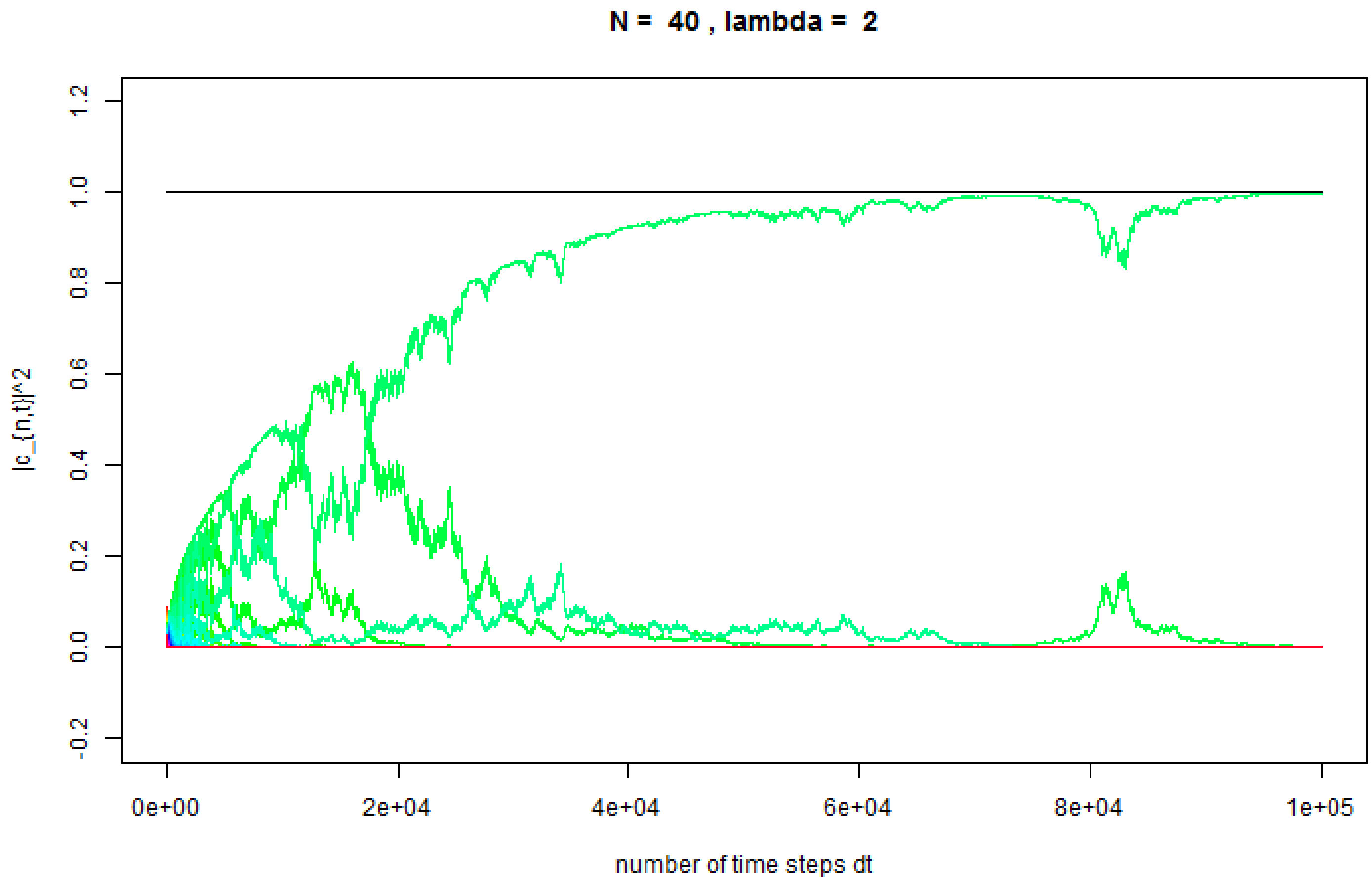
5. A Closer Look at the Postulates: Wave-Collapse Models

- Now N = 40 instead of N = 4,   lambda = 2 :   still T = 1



5. A Closer Look at the Postulates: Wave-Collapse Models

- N = 40 instead of N = 4,   lambda = 2, different random numbers



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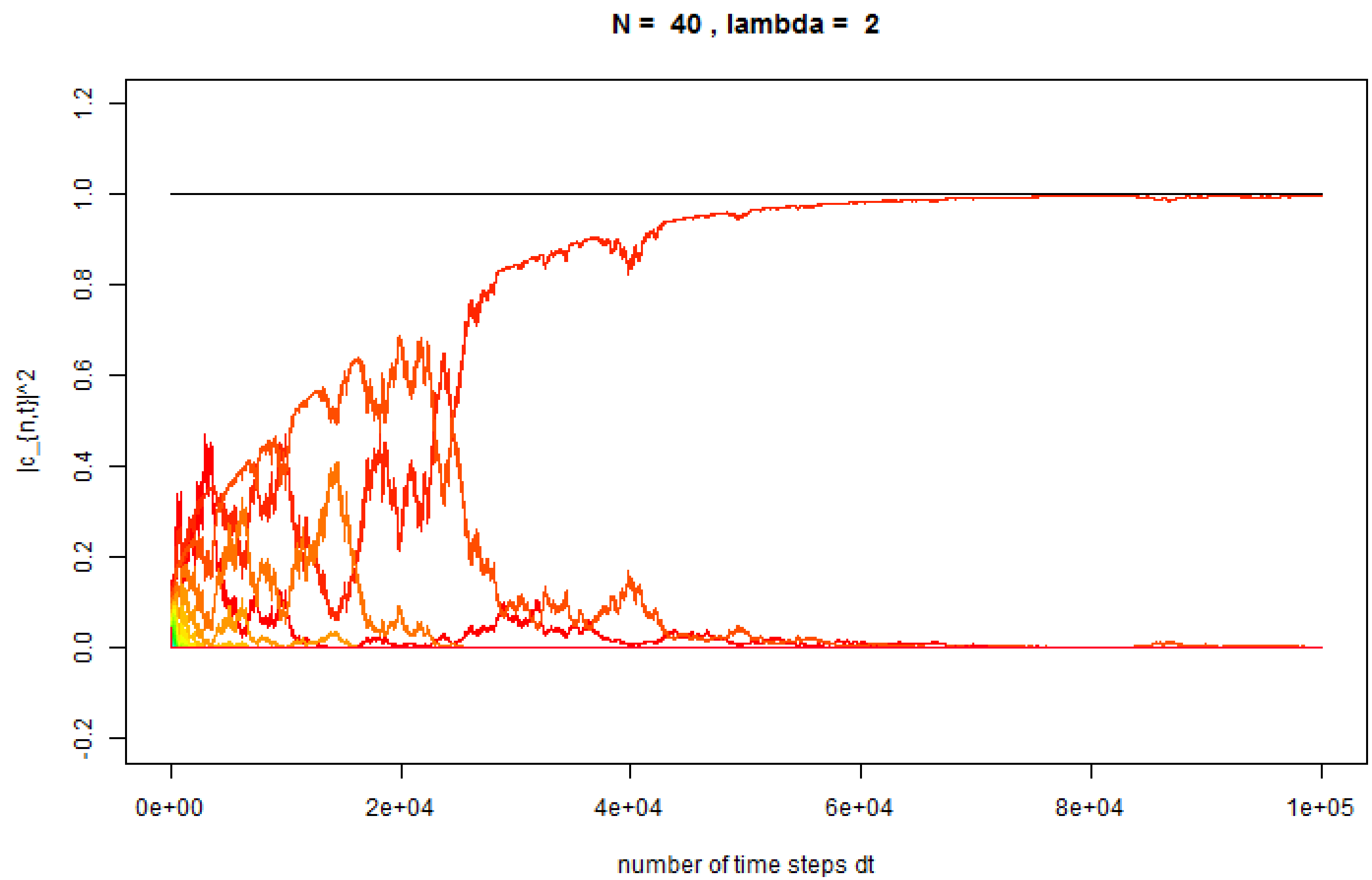
- N = 40 instead of N = 4,   lambda = 2, different random numbers



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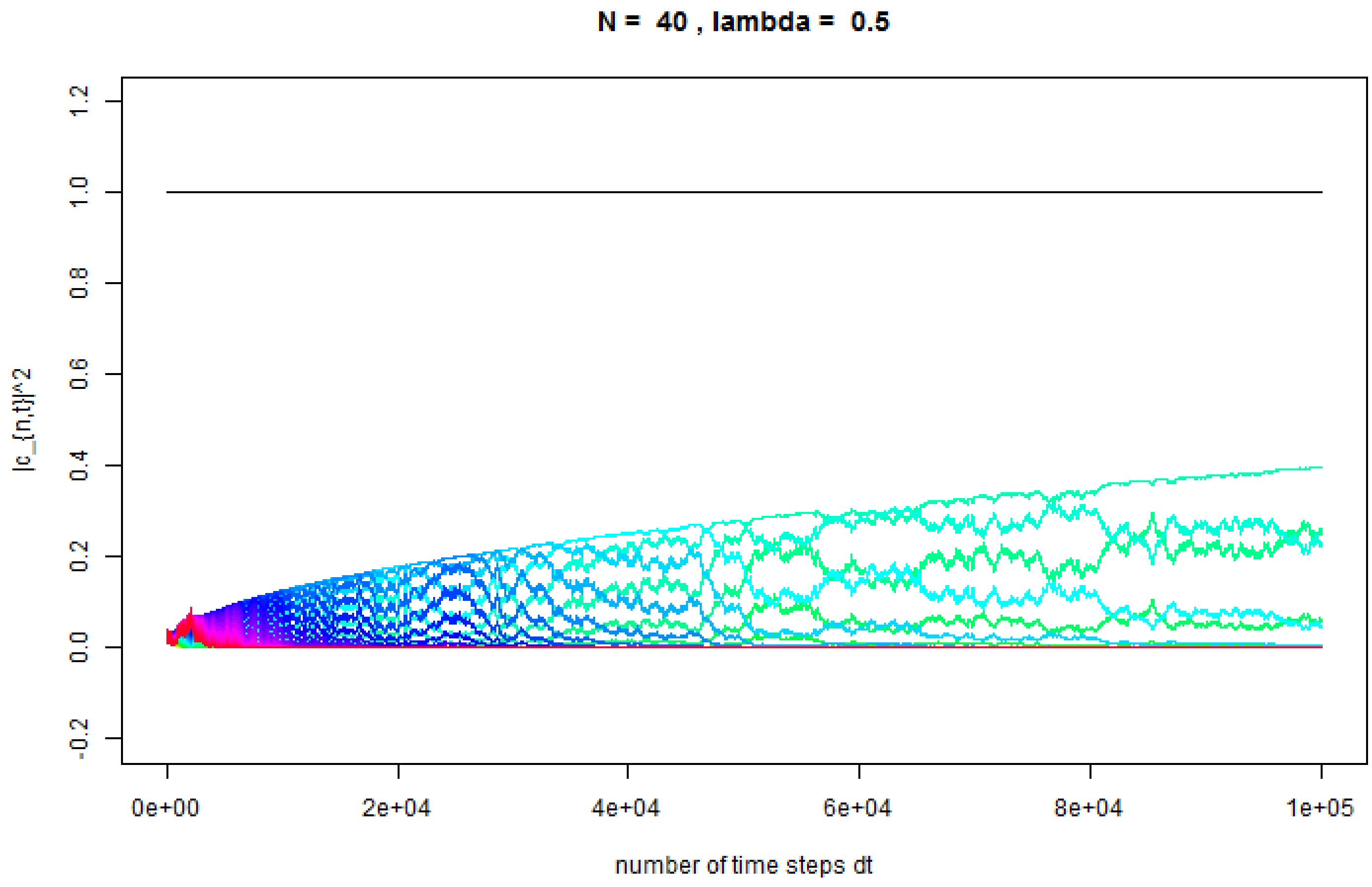
- N = 40, now lambda smaller, lambda = 0.5



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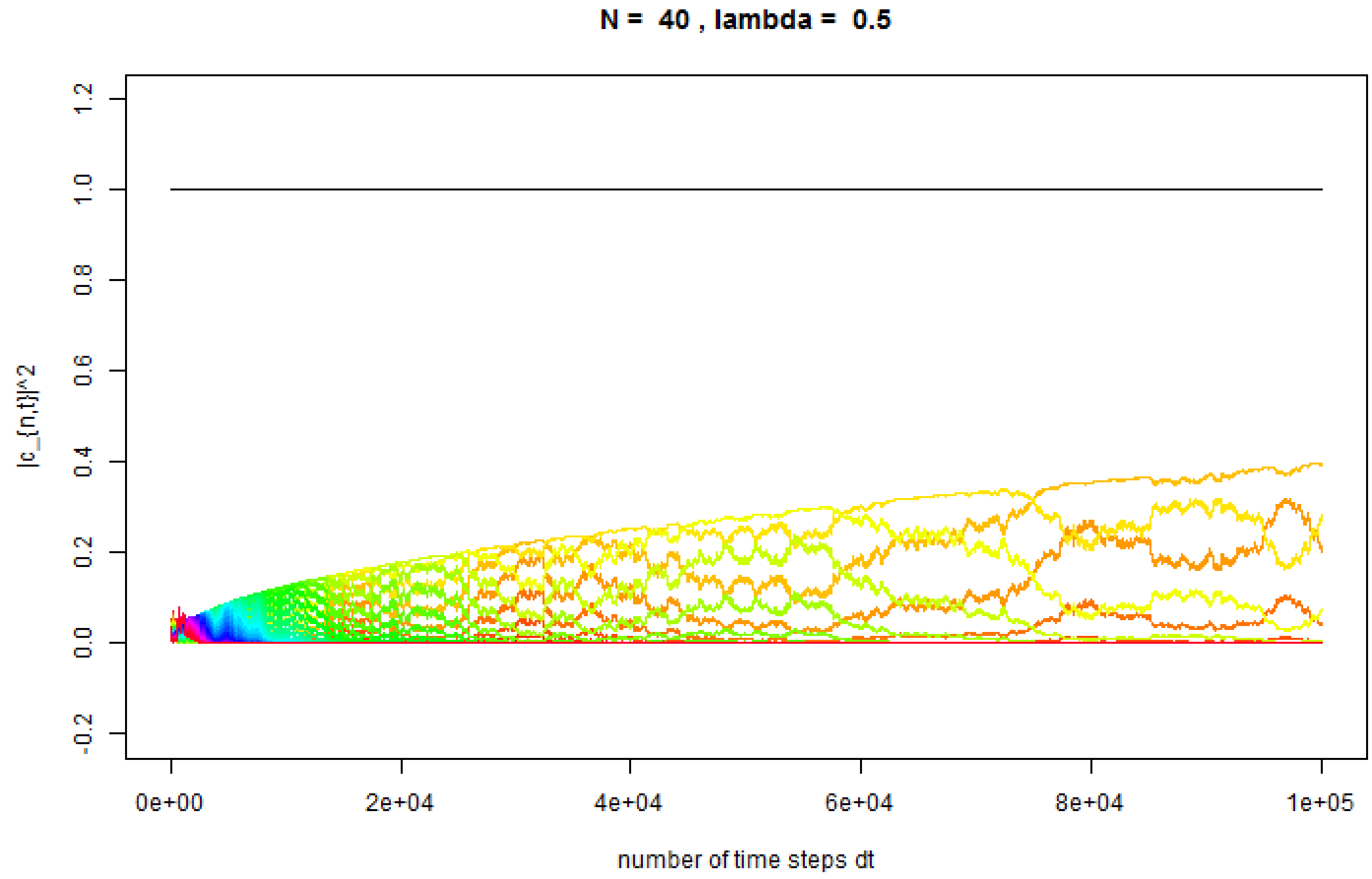
- N = 40, lambda = 0.5, different random numbers



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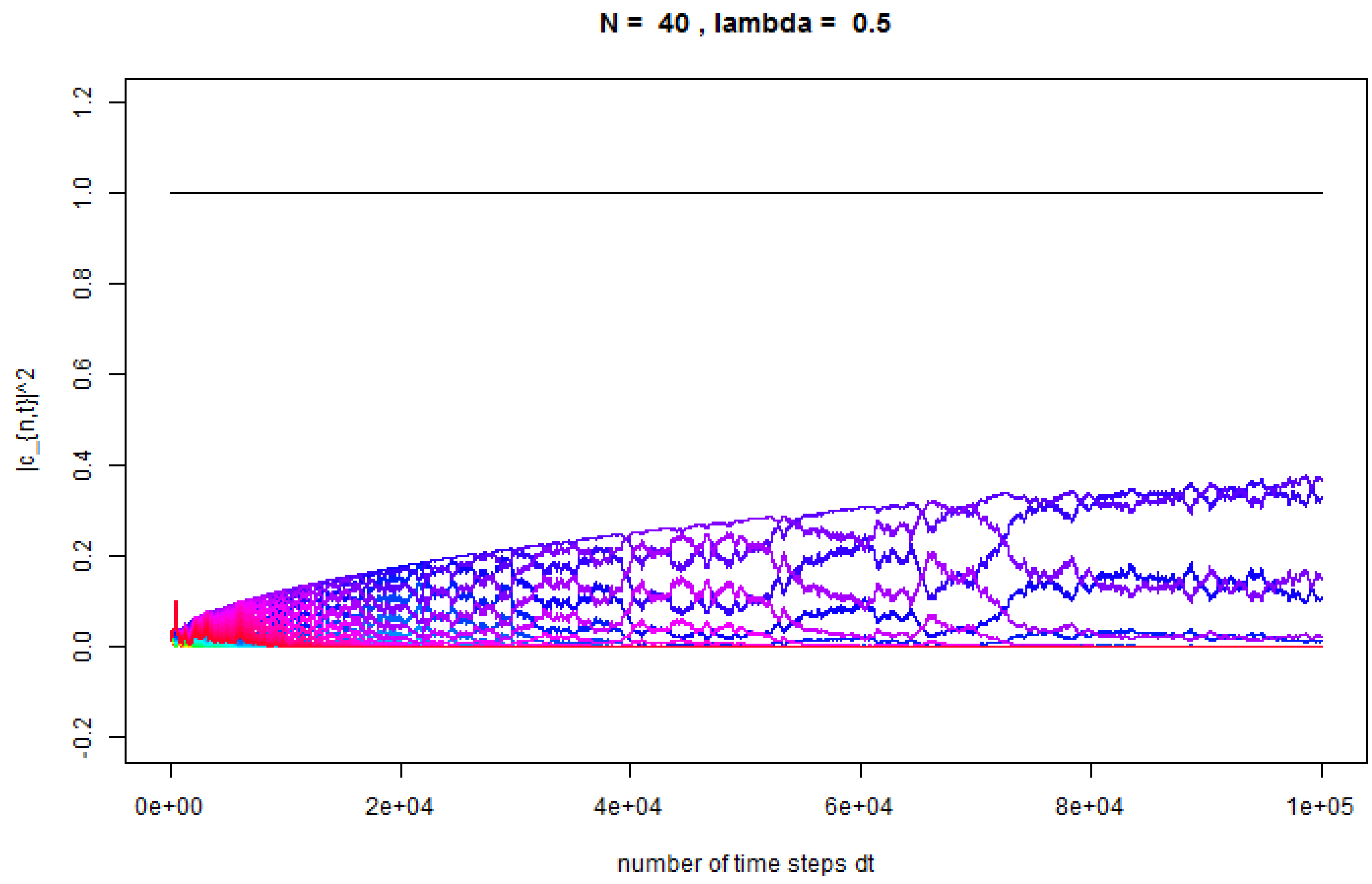
- N = 40, lambda = 0.5, different random numbers



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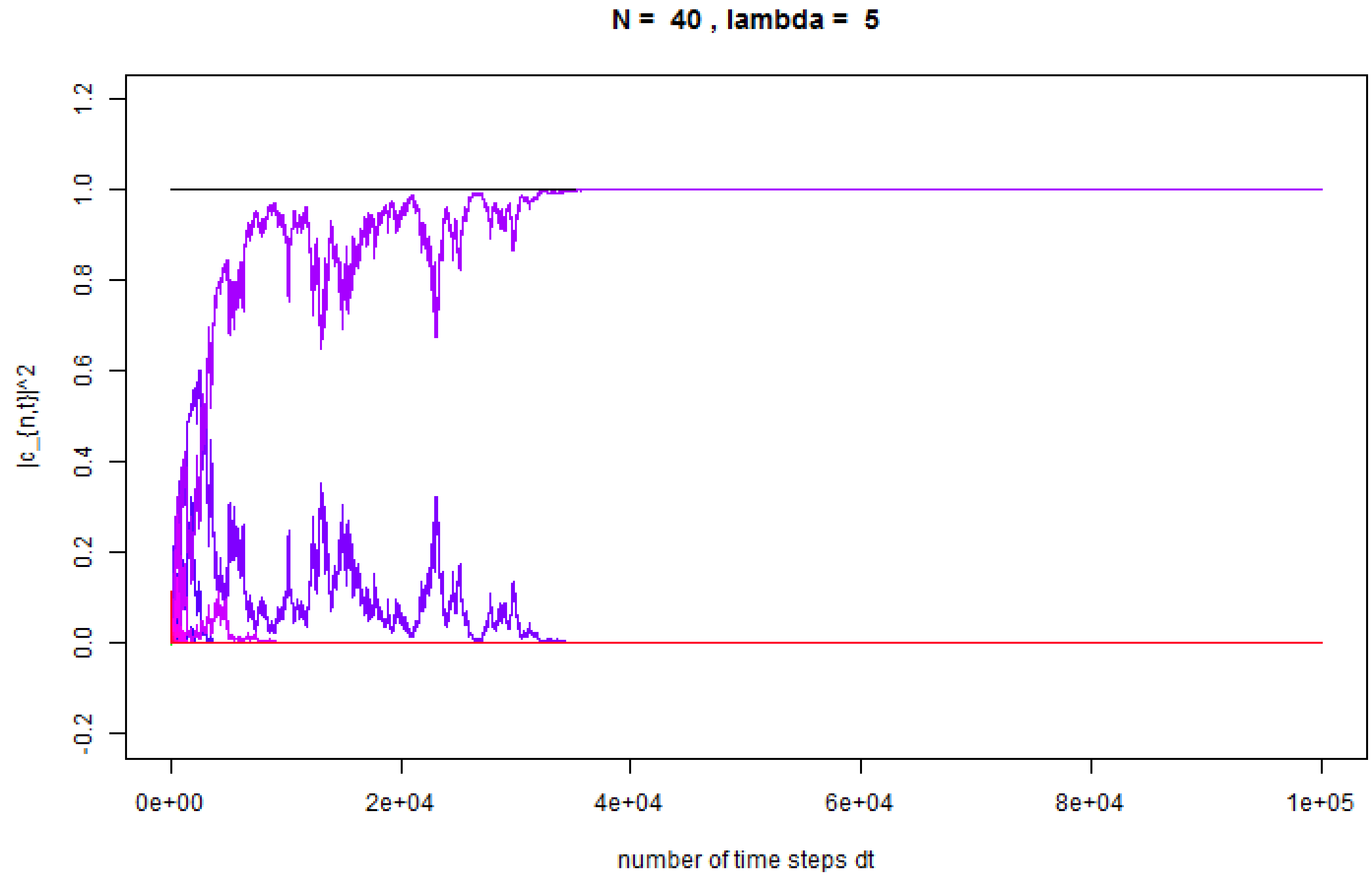
- N = 40, now lambda larger, lambda = 5



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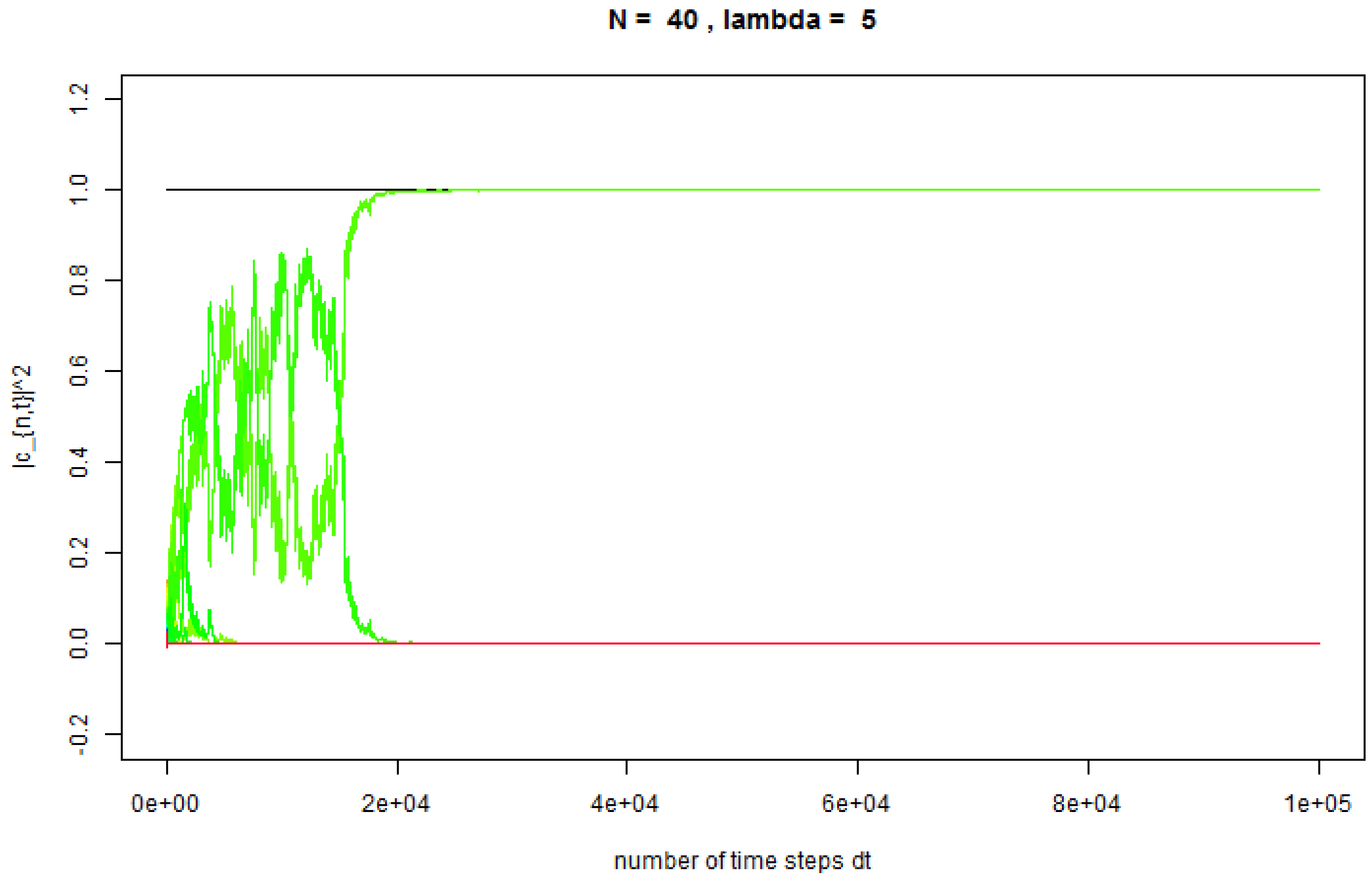
- N = 40, lambda = 5, different random numbers



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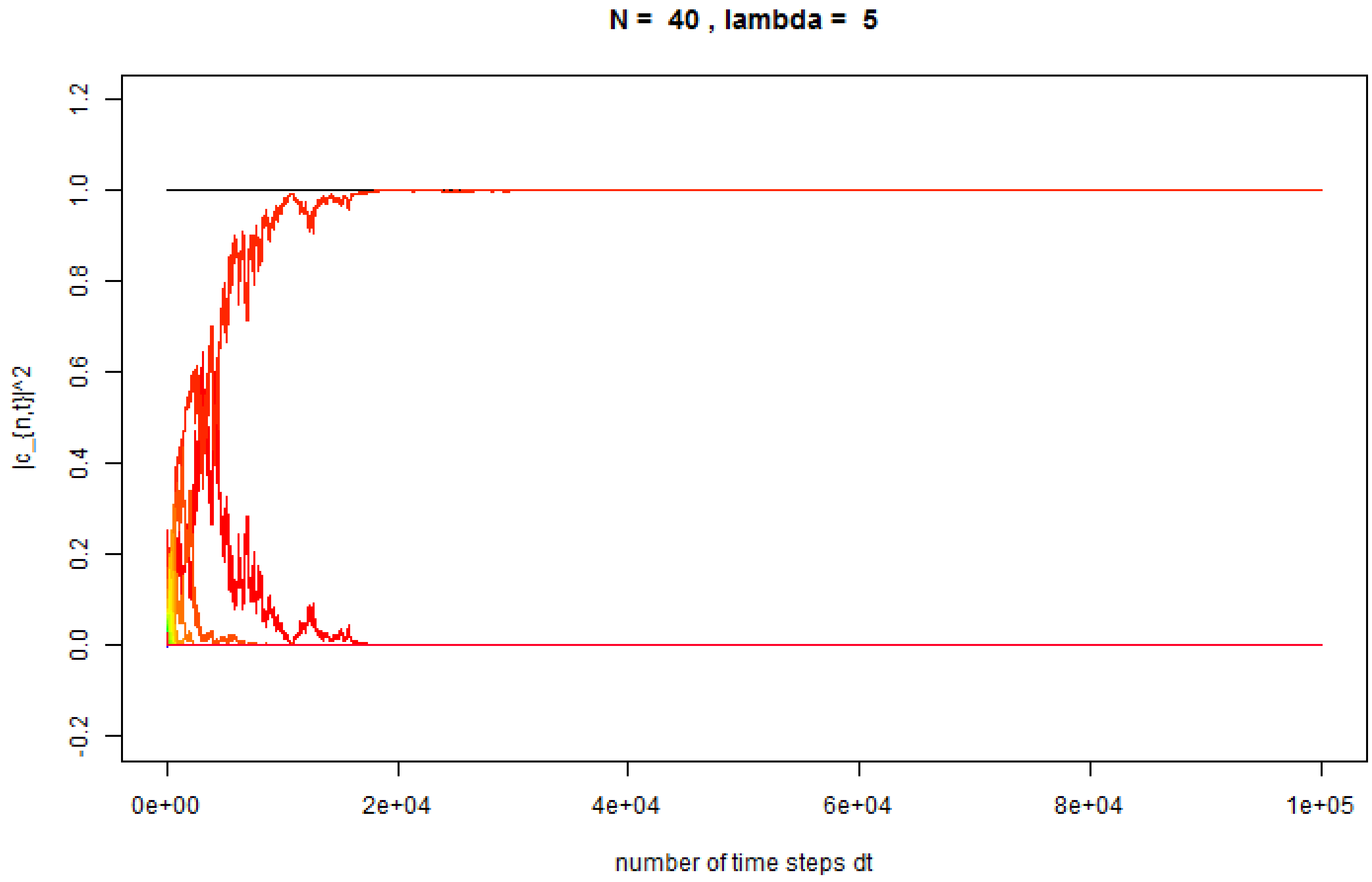

Thank you for your attention!