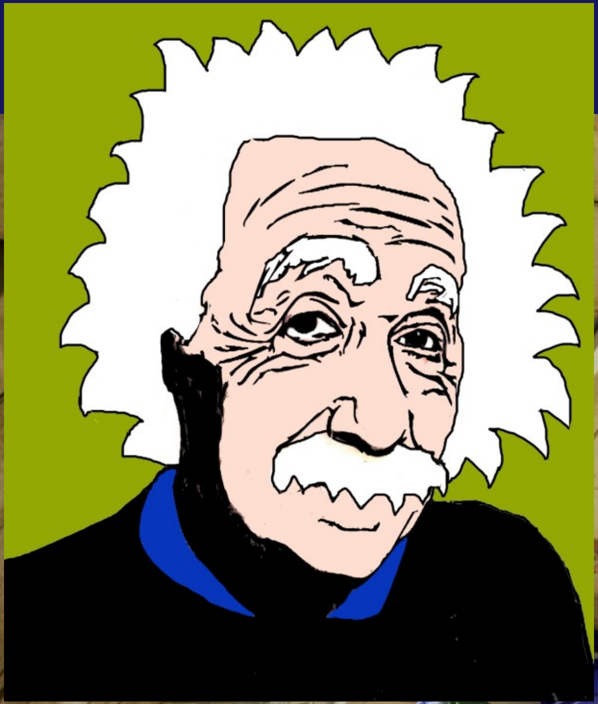


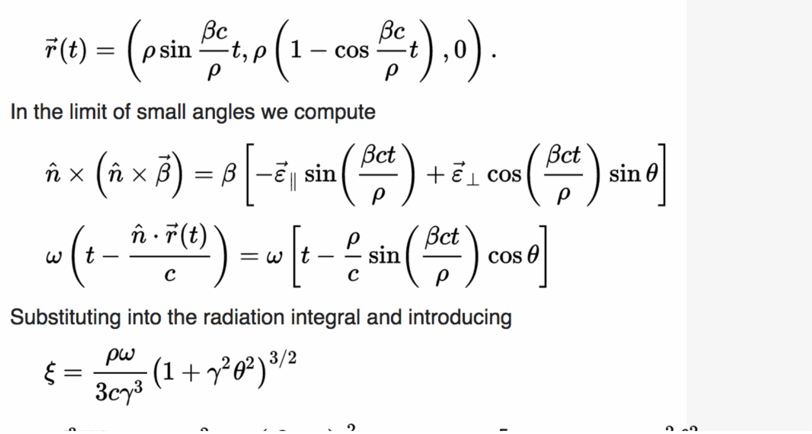
Science@FELs 2020

14-16 September 2020 | Hamburg, Germany

FEL Basics, Generation and Applications

Giorgio Margaritondo
Ecole Polytechnique Fédérale de Lausanne (EPFL)

…to understand free electron lasers, we must first understand synchrotron sources



$$\vec{r}(t) = \left(\rho \sin\frac{\beta c}{\rho}t, \rho\left(1 - \cos\frac{\beta c}{\rho}t\right), 0\right).$$

In the limit of small angles we compute

$$\hat{n} \times \left(\hat{n} \times \vec{\beta}\right) = \beta\left[-\vec{\varepsilon}_{\parallel} \sin\left(\frac{\beta ct}{\rho}\right) + \vec{\varepsilon}_{\perp} \cos\left(\frac{\beta ct}{\rho}\right) \sin\theta\right]$$

$$\omega\left(t - \frac{\hat{n} \cdot \vec{r}(t)}{c}\right) = \omega\left[t - \frac{\rho}{c} \sin\left(\frac{\beta ct}{\rho}\right) \cos\theta\right]$$

Substituting into the radiation integral and introducing

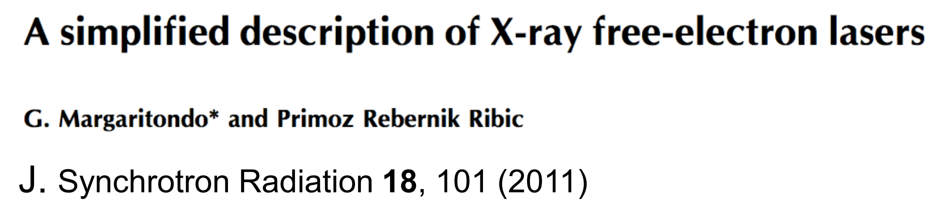
$$\xi = \frac{\rho\omega}{3c\gamma^3}\left(1 + \gamma^2\theta^2\right)^{3/2}$$

…but: must they be so formal and complicated?

J. Synchrotron Rad. (1995). **2**, 148–154

A Primer in Synchrotron Radiation: Everything You Wanted to Know about SEX (Synchrotron Emission of X-rays) but Were Afraid to Ask

G. Margaritondo

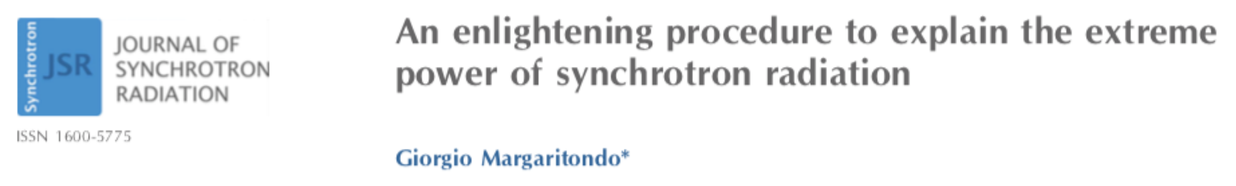


A simplified description of X-ray free-electron lasers

G. Margaritondo* and Primoz Rebernik Ribic

J. Synchrotron Radiation **18**, 101 (2011)

NO!!! We must look at the underlying mechanisms, which are amazingly simple!



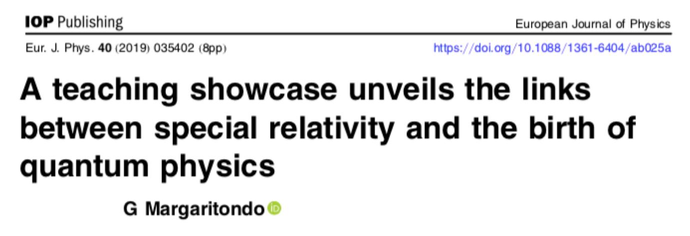
JOURNAL OF SYNCHROTRON RADIATION

ISSN 1600-5775

An enlightening procedure to explain the extreme power of synchrotron radiation

Giorgio Margaritondo*

…an ongoing discovery

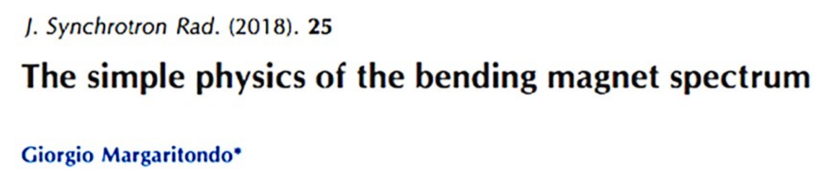


IOP Publishing European Journal of Physics

Eur. J. Phys. **40** (2019) 035402 (8pp) https://doi.org/10.1088/1361-6404/ab025a

A teaching showcase unveils the links between special relativity and the birth of quantum physics

G Margaritondo

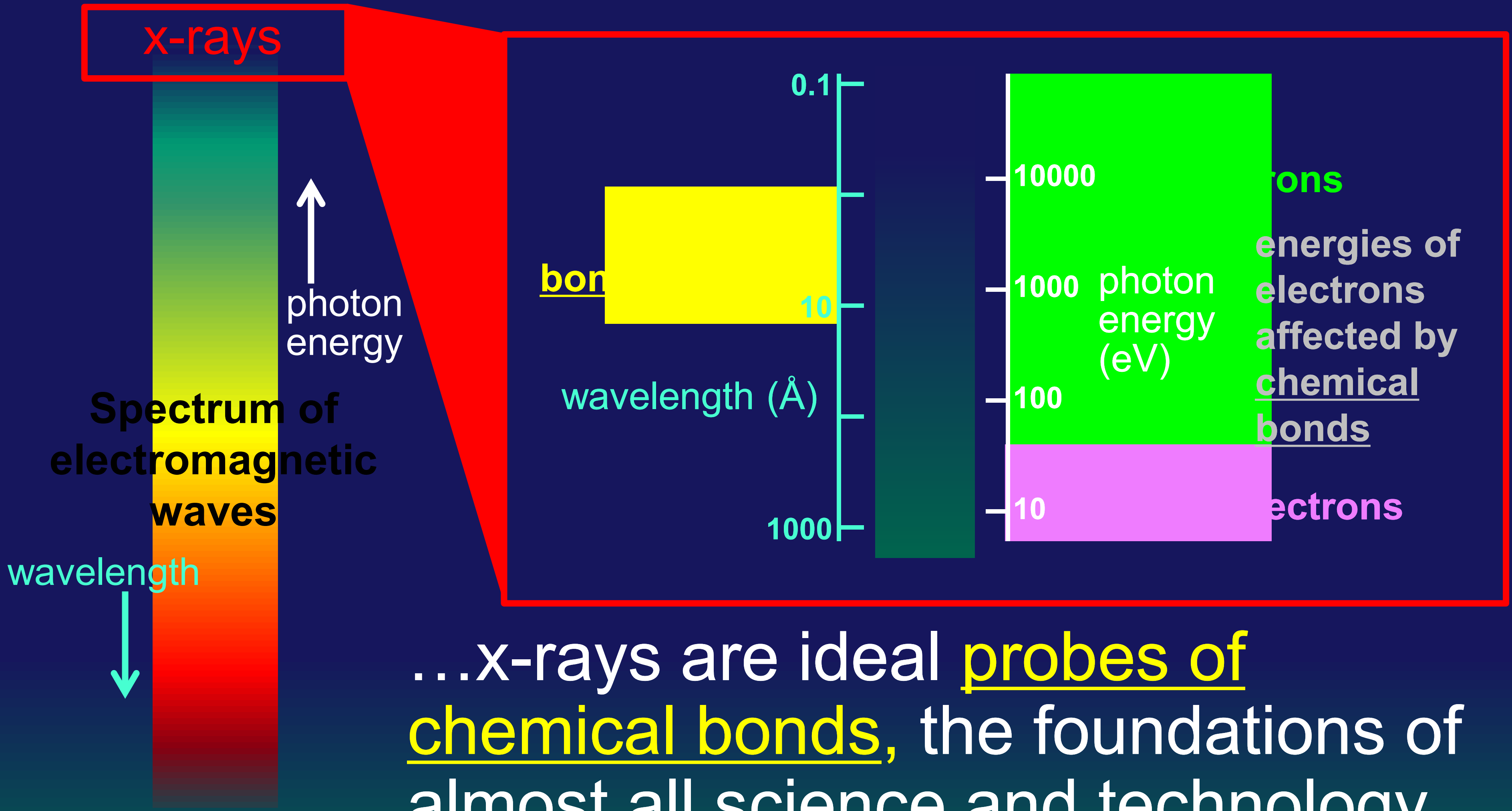


J. Synchrotron Rad. (2018). **25**

The simple physics of the bending magnet spectrum

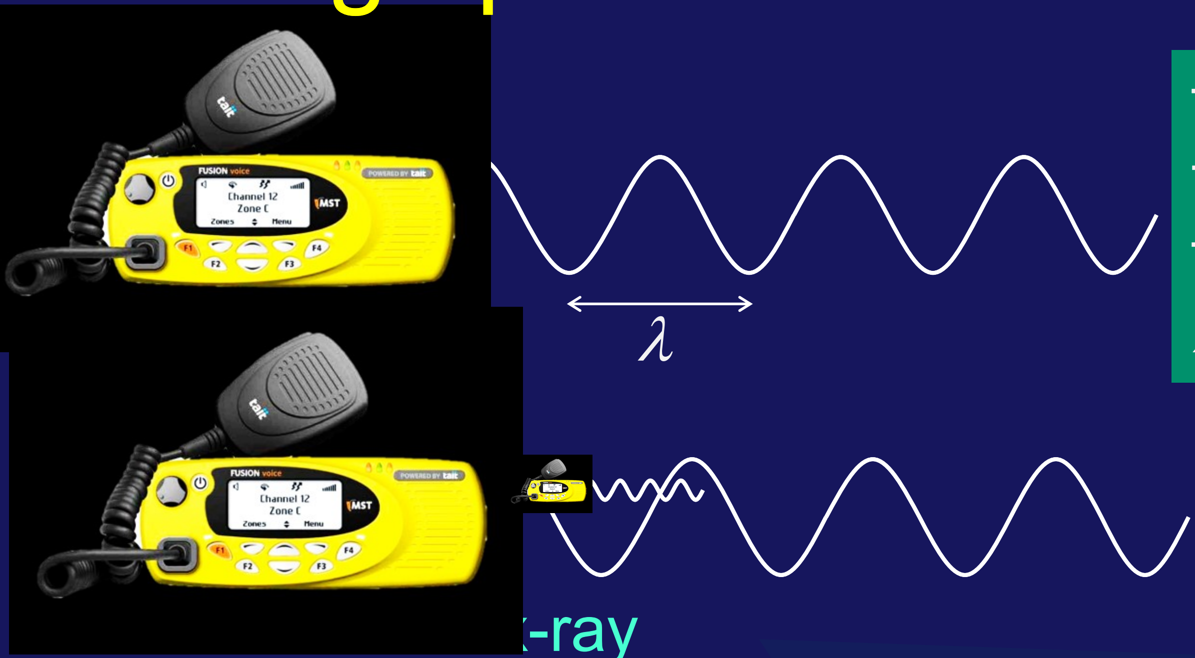
Giorgio Margaritondo*

First: why are x-rays from synchrotrons and FEL's important? What can they probe with their wavelengths and photon energies?



…x-rays are ideal probes of chemical bonds, the foundations of almost all science and technology

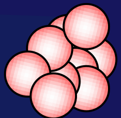
But: building good x-ray sources is a huge problem …and a paradox!



for VHF radio waves, the source size is not far from the wavelength, $\lambda \approx$ 1 meter

-ray wavelengths, the source should shrink to ≈1 Å: one atom

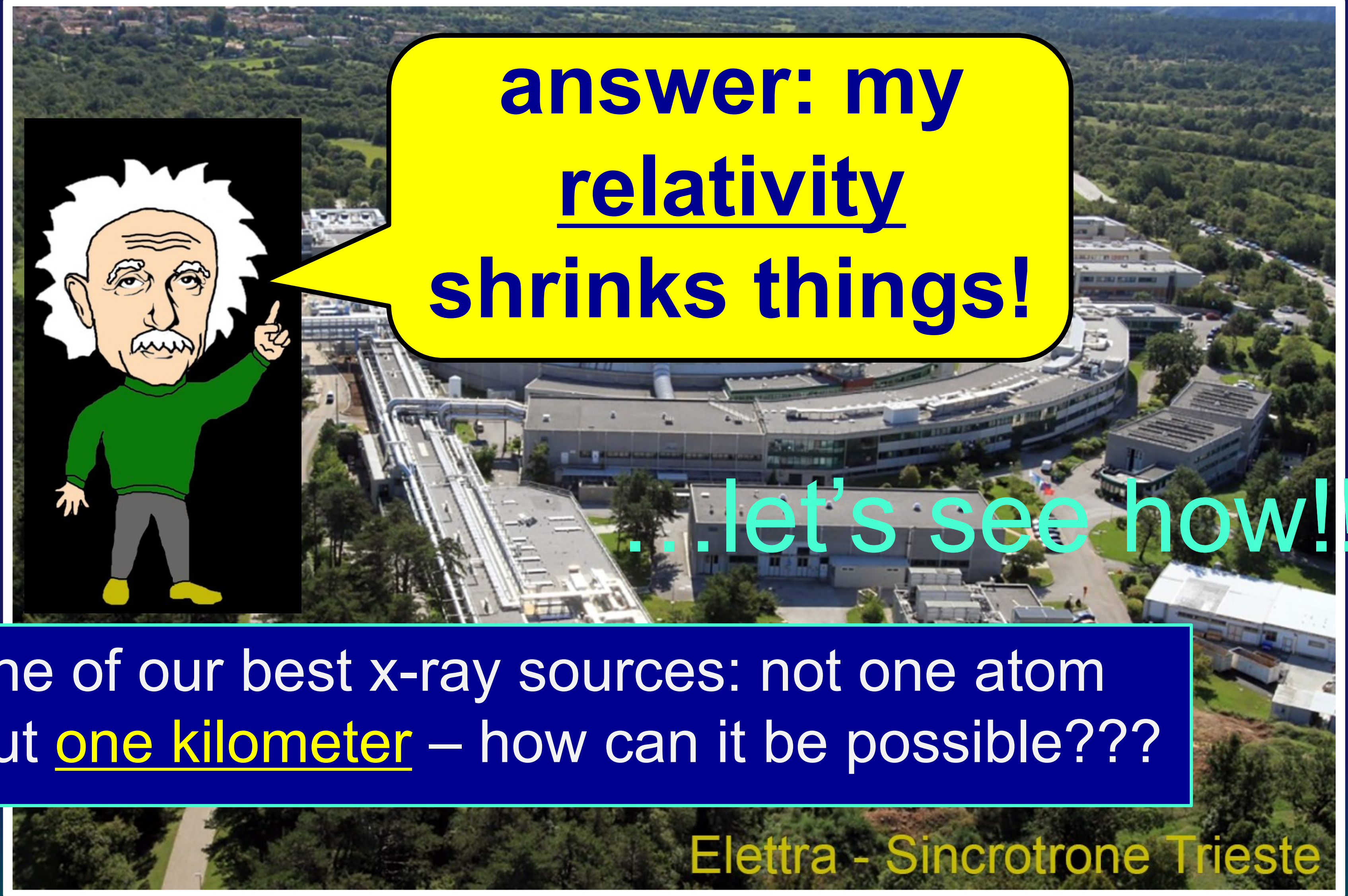
weak flux, large spread



indeed, atoms are the emitters in conventional sources, which are very bad

For better sources, we should build artificial devices with size ≈1 angstrom: no way!

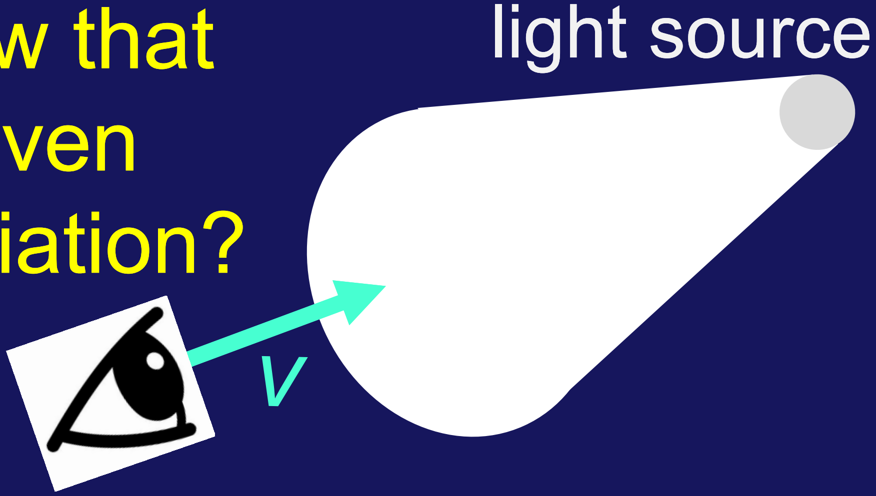
…instead, this is what we use:



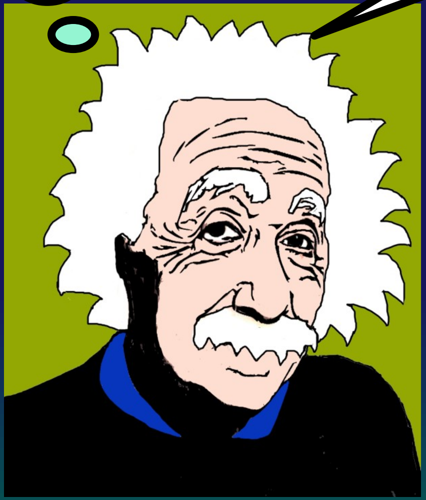
one of our best x-ray sources: not one atom but one kilometer – how can it be possible???

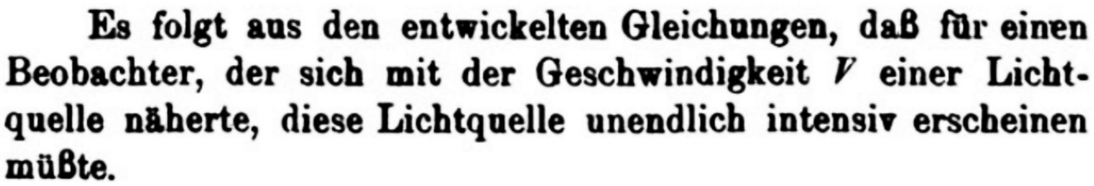
…let’s see how!!!

…by the way: do you know that Albert Einstein, in 1905, even predicted synchrotron radiation?



$$\mathit{Intensity}_{\mathrm{observer}} = \frac{1+v/c}{1-v/c}\,\mathit{Intensity}_{\mathrm{source}}$$





Es folgt aus den entwickelten Gleichungen, daß für einen Beobachter, der sich mit der Geschwindigkeit V einer Lichtquelle näherte, diese Lichtquelle unendlich intensiv erscheinen müßte.

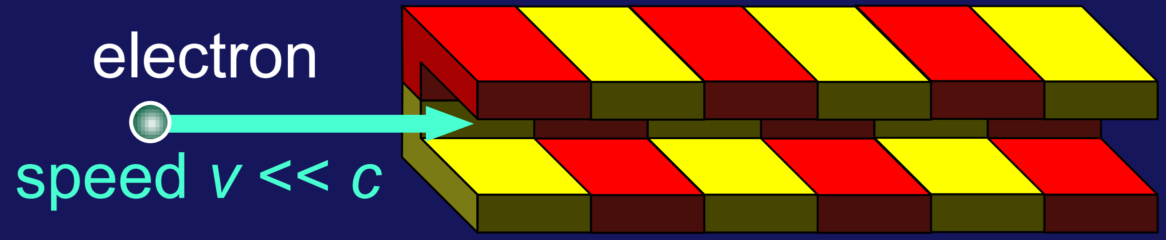
“to an observer approaching a source of light with velocity c, this source of light must appear of infinite intensity”

Let us see now how relativity shrinks synchrotron radiation wavelengths, with a combination of two effects

Start from classical physics: to emit x-rays (electromagnetic waves), we must accelerate a charge

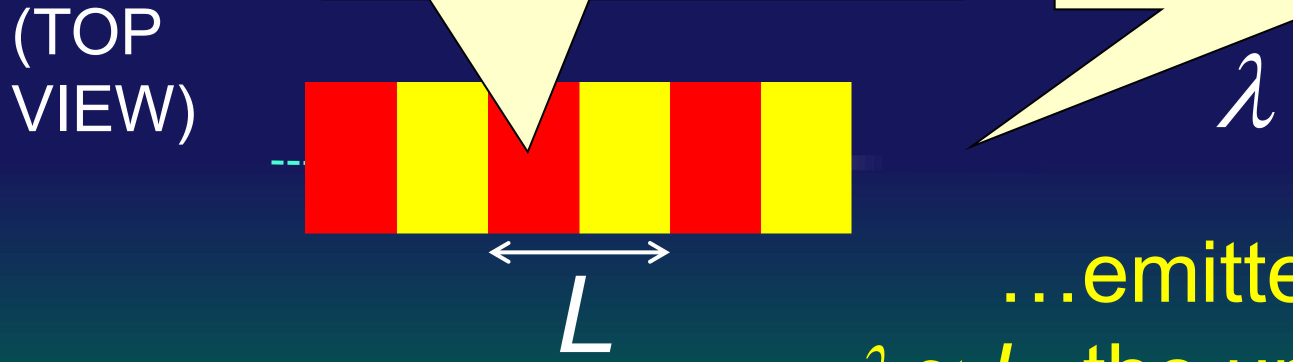
Take an electron: charged and with a small mass → easy to accelerate

Assume that the electron travels at non-relativistic speed through a periodic series of magnets ("undulator")



The undulator forces the electron to oscillate in the transverse direction

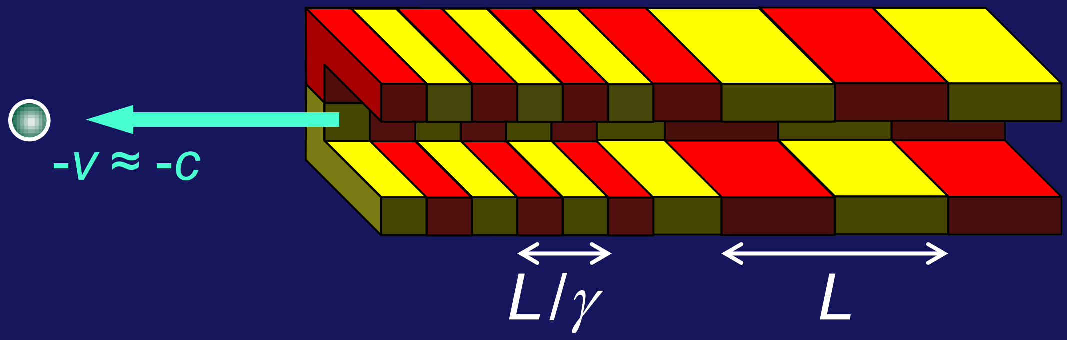
…and, due to transverse acceleration, to emit electromagnetic waves



…emitted wavelength:
$\lambda \approx L$, the undulator period

Now consider a relativistic electron, with speed $v \approx c$

The electron "sees" the undulator arriving with velocity $-v \approx -c$



…and the emitted wavelength decreases, because the electron "sees" L shrunk by the relativistic <u>Lorentz contraction</u>, to $\approx L/\gamma$

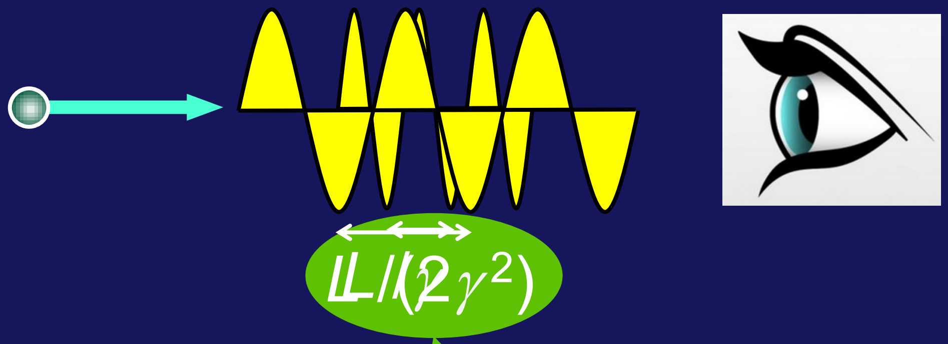
$$\text{where } \gamma = \frac{1}{\sqrt{1-v^2/c^2}} = \frac{\text{energy}}{m_o c^2}$$

$v \approx c \rightarrow$ large $\gamma \rightarrow$ small L/γ

typically, energy = several GeV, $m_o c^2 \approx 0.5$ MeV,

$\gamma = 2000 - 12{,}000$

Indeed, L/γ is the emitted wavelength seen in the electron reference frame…



…but in the laboratory frame the motion of the source (the electron) causes the relativistic Doppler effect -- further decreasing the detected wavelength by a factor $\approx 1/(2\gamma)$

Together, the Doppler effect and the Lorentz contraction decrease the wavelength to:

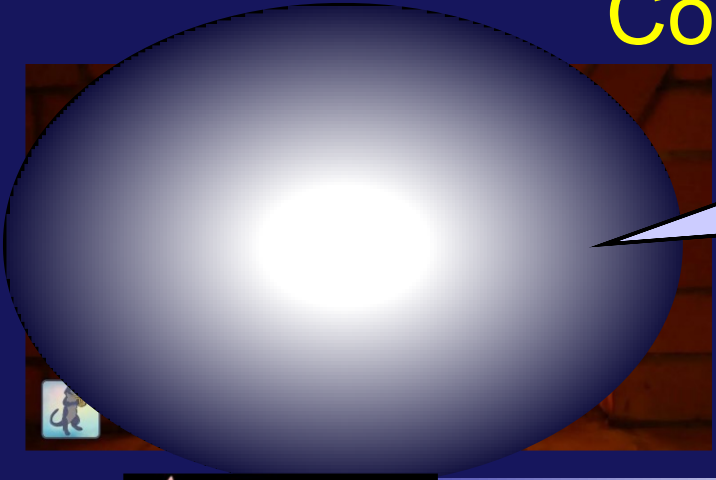
$$\lambda \approx \frac{L/\gamma}{2\gamma} = \frac{L}{2\gamma^2}$$

Example: L = 1 cm, γ = 5000 → $\lambda \approx$ 2 Å: x-rays!!!

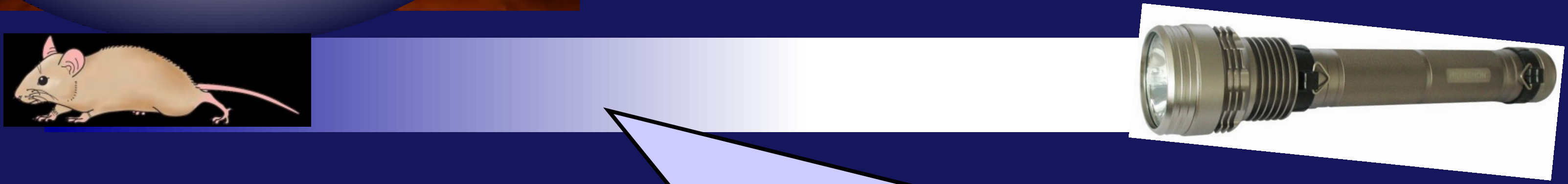
OK, relativistic electrons produce x-rays: but can this give us good x-ray sources?

First: what is a “good” x-ray source?

Consider fireplaces and flashlights



A fireplace is not very effective in illuminating a target: its emission is from a large area and spread over a broad solid angle



A flashlight is much more effective, being a small-area source with a narrow angular spread

This leads us to the notion of “brightness” (or “brilliance”)

The "brightness" (or "brilliance") measures the quality of a source of waves, including x-rays:

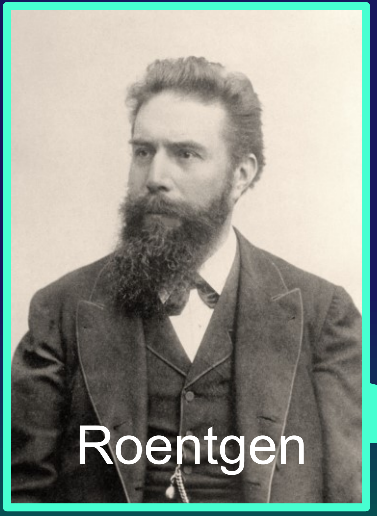
$$\boxed{\text{Brightness} = \text{constant}\ \frac{F}{\xi^2\,\Omega}}$$

Small ξ and $\Omega \Rightarrow$ high brightness: a large flux is good, but geometry also matters

History of x-ray sources: synchrotron radiation boosted the brightness

(units: photons/mm^2/s/mrad^2, 0.1% bandwidth)

an increase by 26 orders of magnitude since 1970, while computer chips "only" improved by 7 orders of magnitude!!!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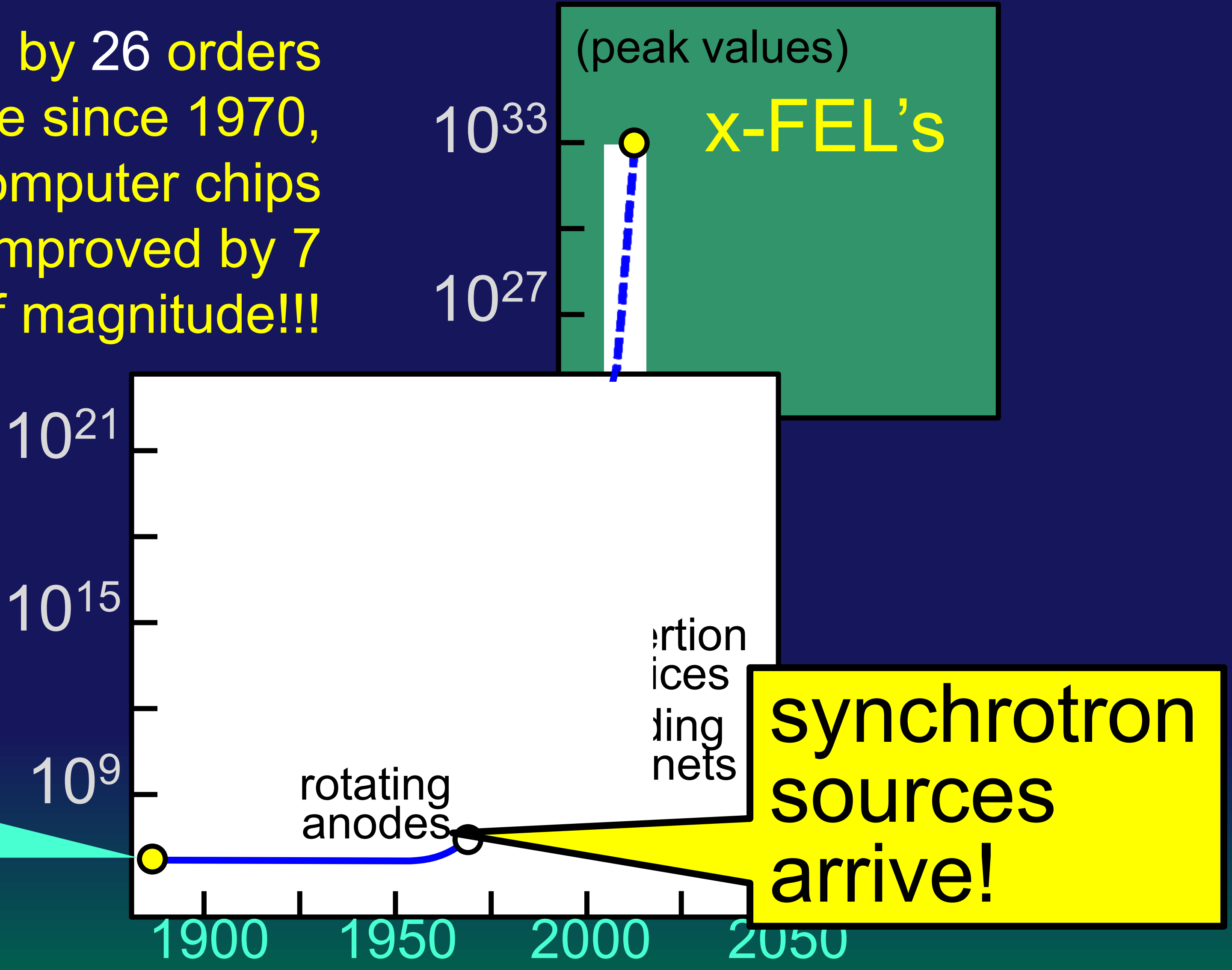


synchrotron sources arrive!

What brings synchrotron sources to extremely high brightness?

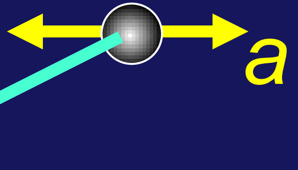
Four factors:

1. Electrons in vacuum can emit more power than electrons in a solid since the power does not damage their environment
   $\Rightarrow$ high flux

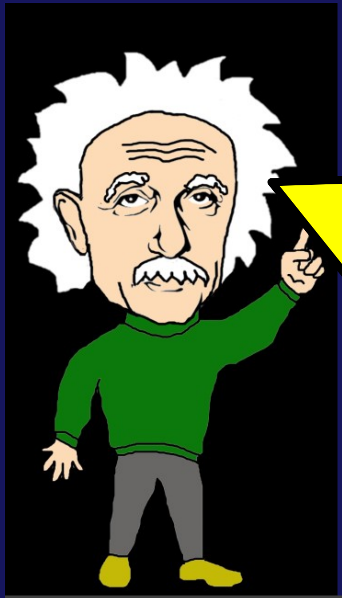
2. Different electrons circulate in the accelerator along slightly different paths. The source size is the transverse cross section of all paths. Sophisticated electron beam controls make it very small
3. Relativity drastically boosts the **emitted power**
4. Relativity also reduces the **angular divergence**

How does relativity boost the emitted power of a synchrotron source?

The classical (Larmor) emitted power in the electron frame is proportional to a^2 (a = transverse acceleration)



the longitudinal velocity $v \approx c$ makes the electron relativistic

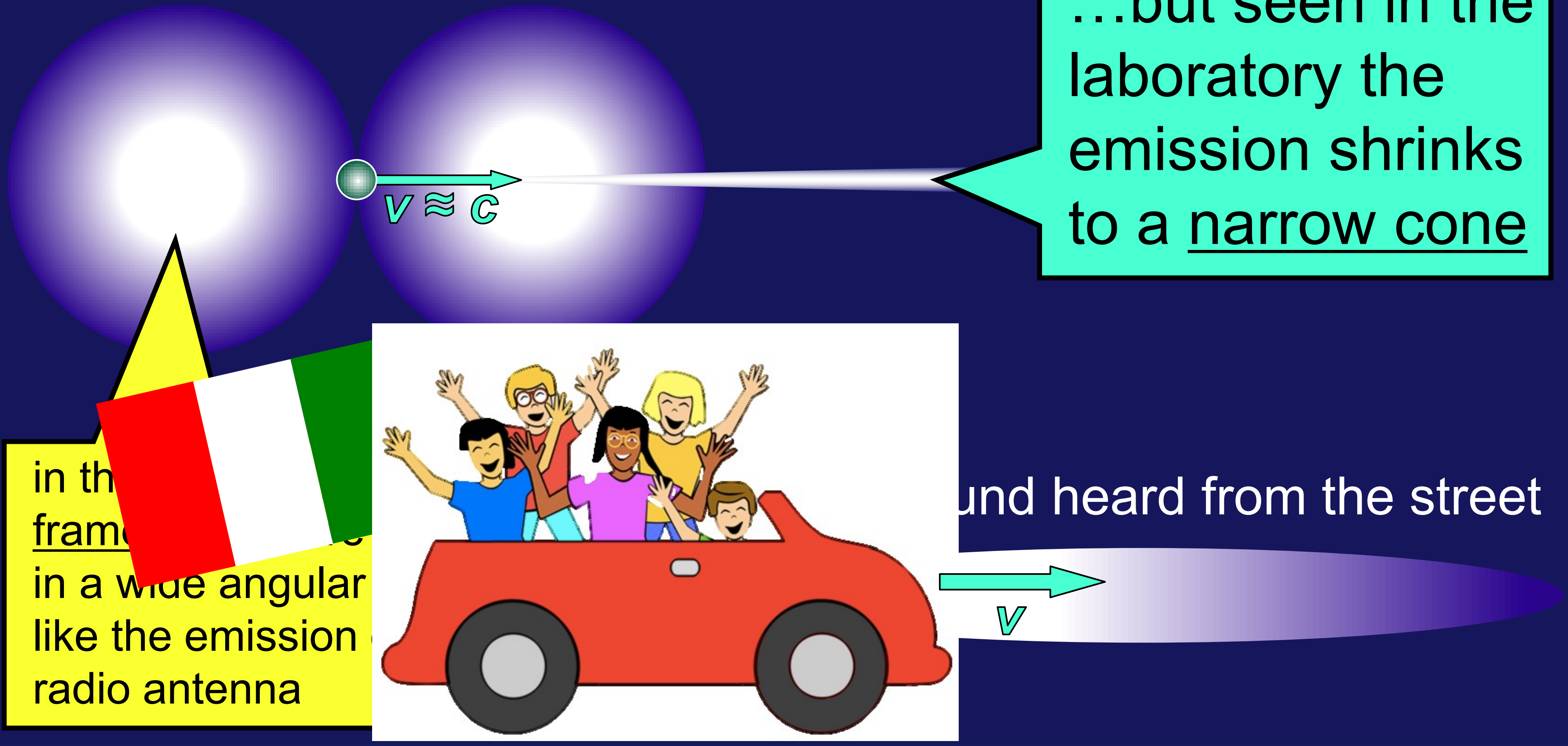


Electron frame → lab frame: the transverse coordinate does not change, and the time t is multiplied by $1/\gamma$; the acceleration a, proportional to $1/t^2$, is multiplied by γ^2, so the emitted power is **proportional to γ^4 = [energy/($m_o c^2$)]^4**

The emission increases with the 4th power of the electron energy, to extremely high levels

The emission decreases as $1/m_o^4$: electrons emit a lot, protons much less

Relativity at work again: the angular collimation of synchrotron radiation



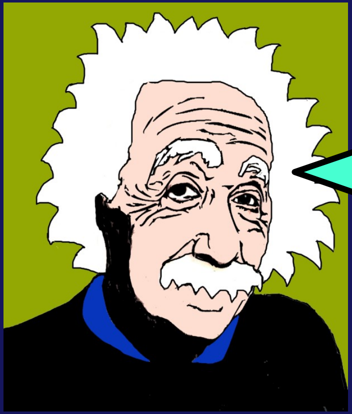
…but seen in the laboratory the emission shrinks to a <u>narrow cone</u>

in th
<u>fram</u>
in a w de angular
like the emission
radio antenna

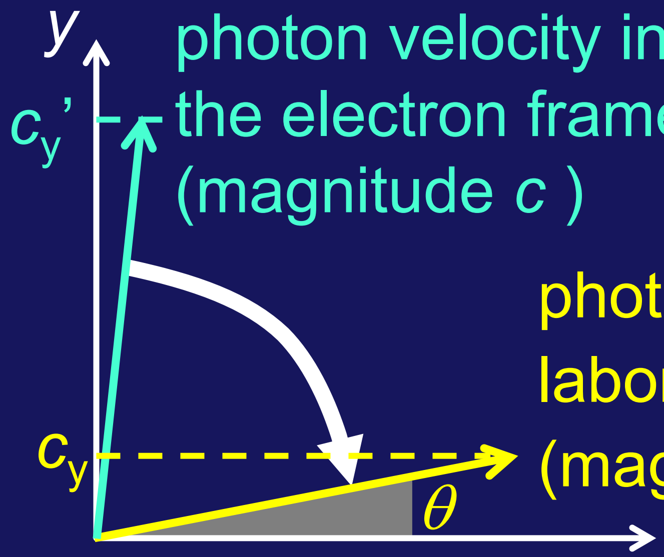
und heard from the street

…like the forward projection of the sound from a car celebrating a victory of the Italian national soccer team -- but <u>made extreme relativity</u>: the electrons behave like **super-narrow flashlights**

The relativistic "flashlight effect" in detail:



A photon is emitted in a transverse direction in the electron frame



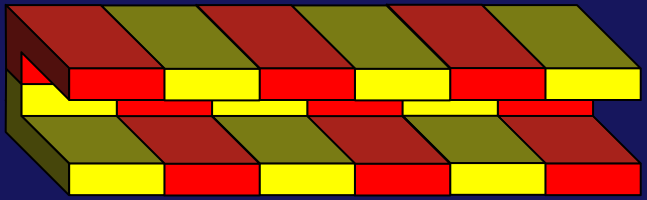
photon velocity in the electron frame (magnitude *c*)

photon velocity in the laboratory frame (magnitude *c*)

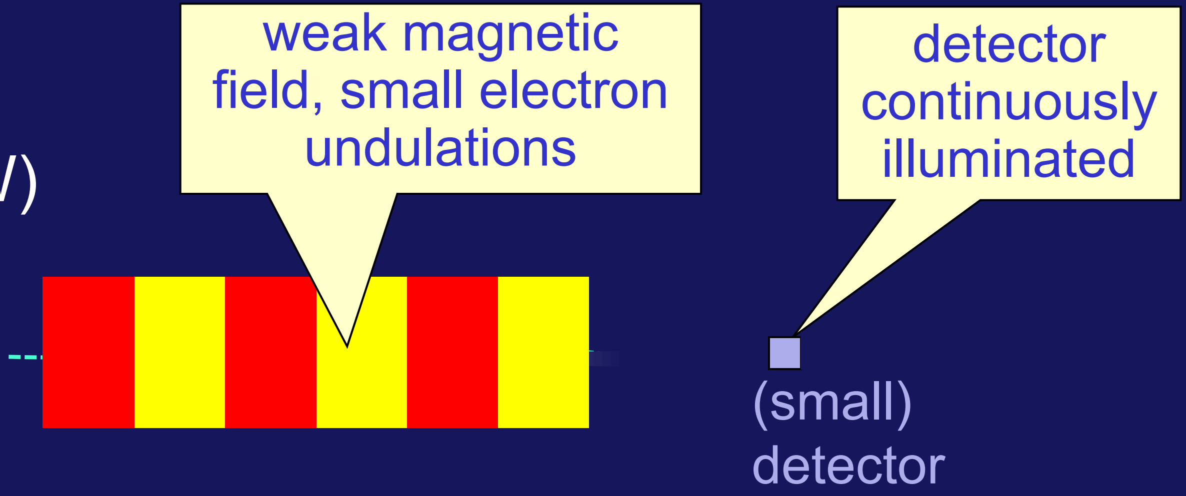
Lorentz transformation from the electron frame to the laboratory frame: the transverse velocity component changes from $c_y' \approx c$ to $c_y = c_y'/\gamma \approx c/\gamma$. The magnitude *c* is invariant, so the velocity vector rotates, to an angle $\theta \approx c_y/c \approx 1/\gamma$ from the forward direction

Spread: $\approx 2\theta \approx 2/\gamma \approx$ microradians: narrow!!!

The "flashlight effect" for undulators:



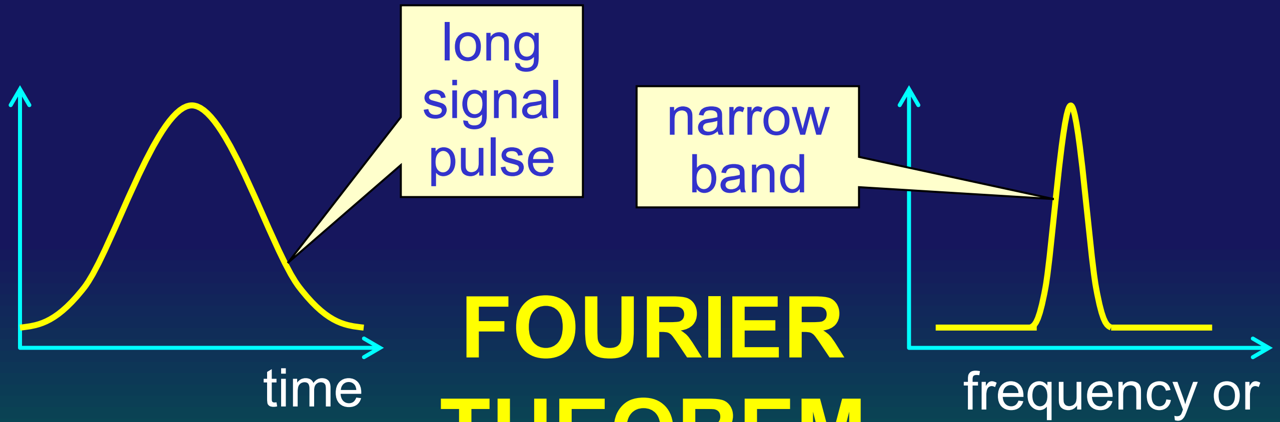
(TOP VIEW)



weak magnetic field, small electron undulations

detector continuously illuminated

(small) detector

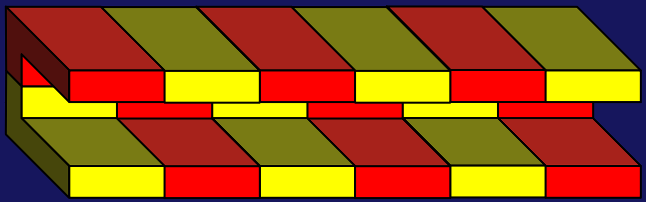


long signal pulse

narrow band

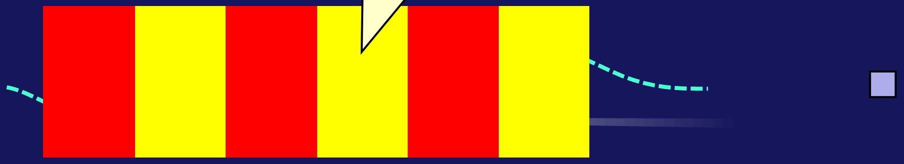
FOURIER THEOREM

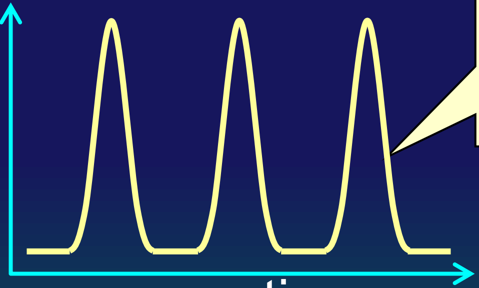
The “flashlight effect” for another type of sources: “wigglers”



Strong magnetic field, large undulations

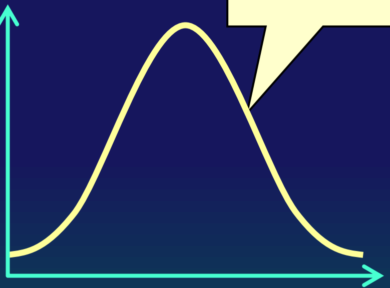
(TOP VIEW)





Series of short pulses

FOURIER THEOREM

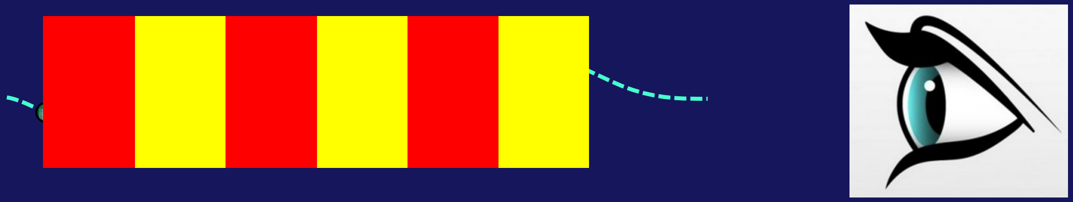


Broad band

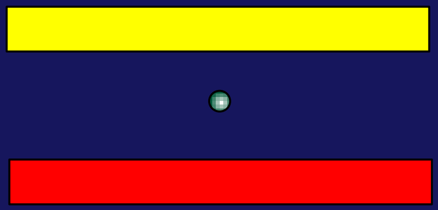
Synchrotron radiation polarization:

An electron in an undulator or a wiggler:

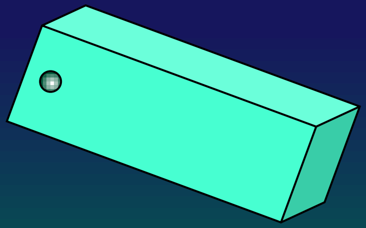
TOP VIEW:



FRONT VIEW:



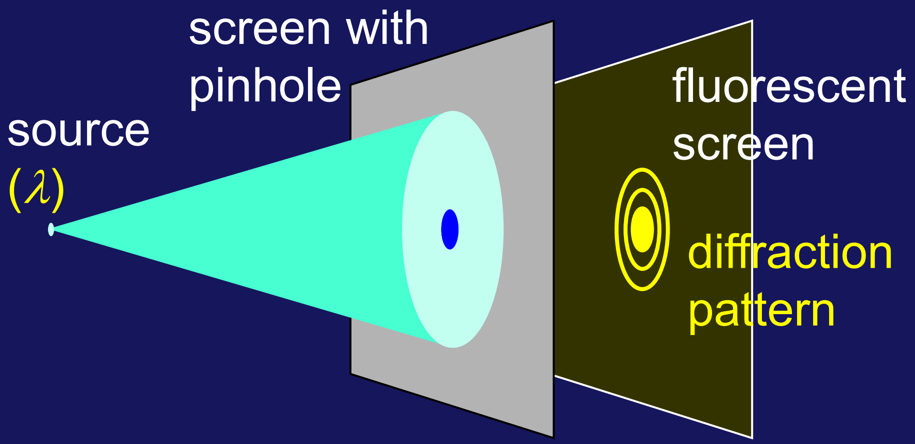
Linear polarization in the horizontal plane – where the electric field perturbations take place



Special (elliptical) wigglers/undulators can produce intense elliptically polarized radiation

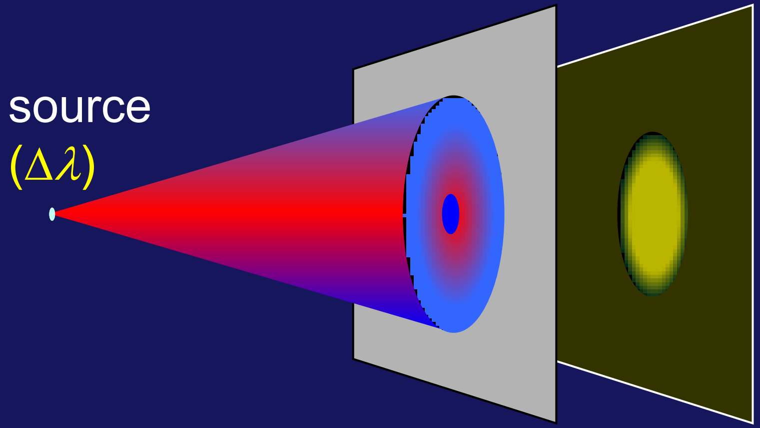
Another important feature: COHERENCE!

"the property that enables radiation to produce visible wave-like (diffraction or interference) effects"

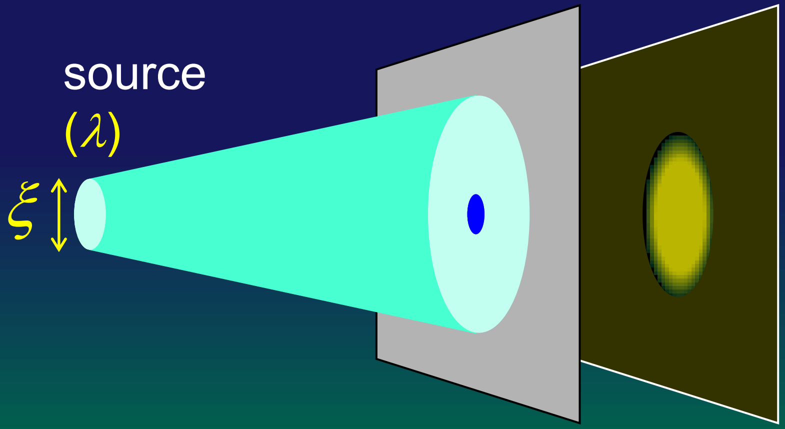


A point source emitting only one wavelength always produces a visible diffraction pattern: it has full coherence

Analyzing realistic sources, we find TWO kinds of coherence: "time" and "spatial"

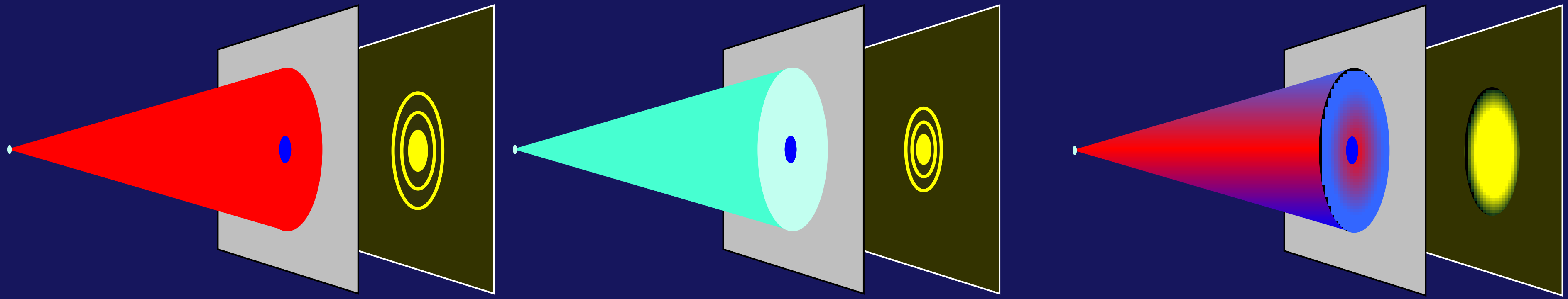


…if the source emits a band of wavelengths, the pattern may no longer be visible: this leads to the notion of "time coherence"



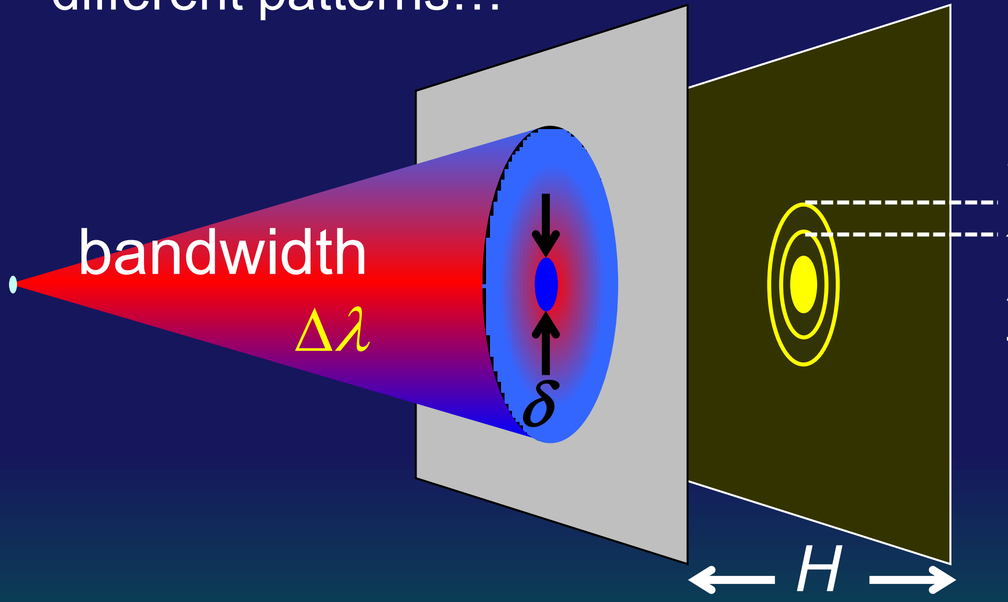
Likewise, if the source has a finite size the pattern may become impossible to see: this leads to "spatial coherence"

Effects of a finite wavelength band: time (longitudinal) coherence



different wavelengths produce different patterns…

…but their superposition may blur the pattern features



spacing between fringes:

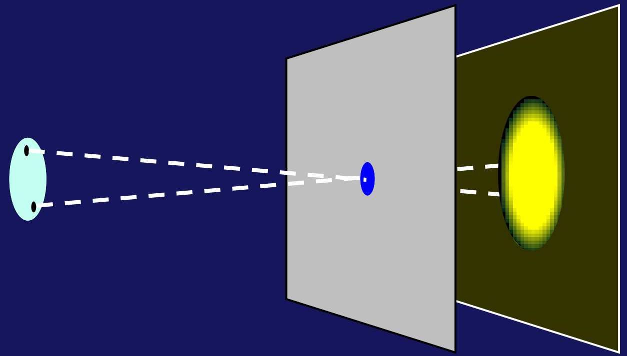
$x \approx (H/\delta)\lambda$

$\Delta\lambda$ “blurs” x to $\Delta x \approx (H/\delta)\Delta\lambda$

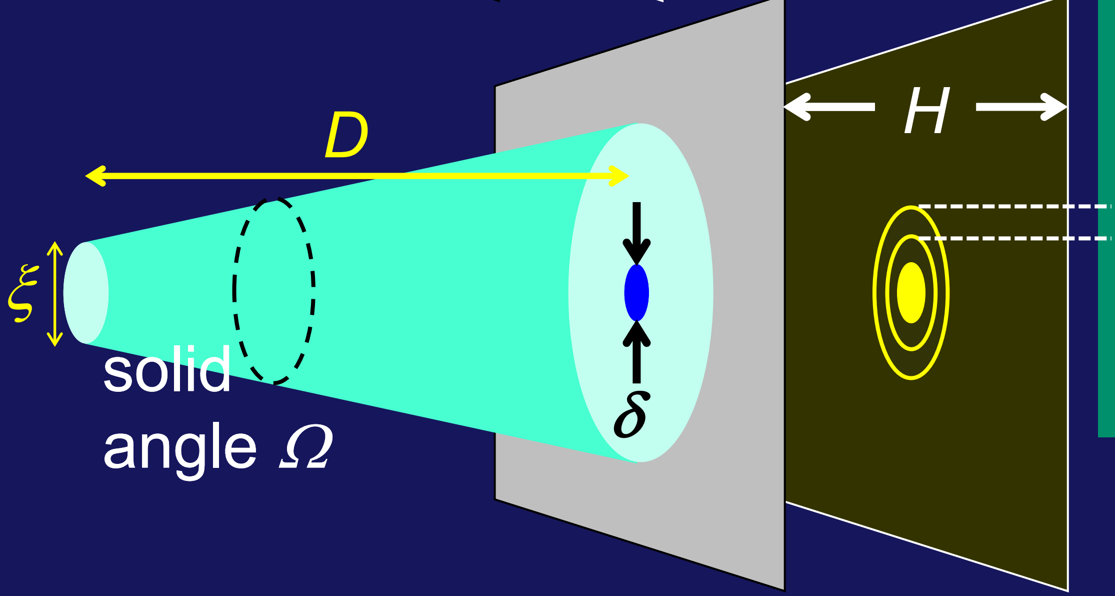
to see the pattern: $\Delta x < x$, $\Delta\lambda/\lambda < 1$

Using the “coherence length” $L_c = \lambda^2/\Delta\lambda$, the condition for time coherence is: $L_c > \lambda$

Source geometry: spatial (lateral) coherence



Each point in the source produces a diffraction pattern – but the superposition may blur the pattern features



When are such features visible?

$\xi H/D \approx$ maximum distance between centers of patterns for different source points

$x \approx (H/\delta)\lambda$ = fringe spacing

To see the pattern features:

$\xi H/D \leq x \rightarrow \boxed{\delta \leq \lambda D/\xi}$

condition for lateral coherence

Another way to analyze lateral coherence:

Illuminated screen area: ΩD^2; pinhole area $\approx \delta^2$; portion of waves that contribute to diffraction:

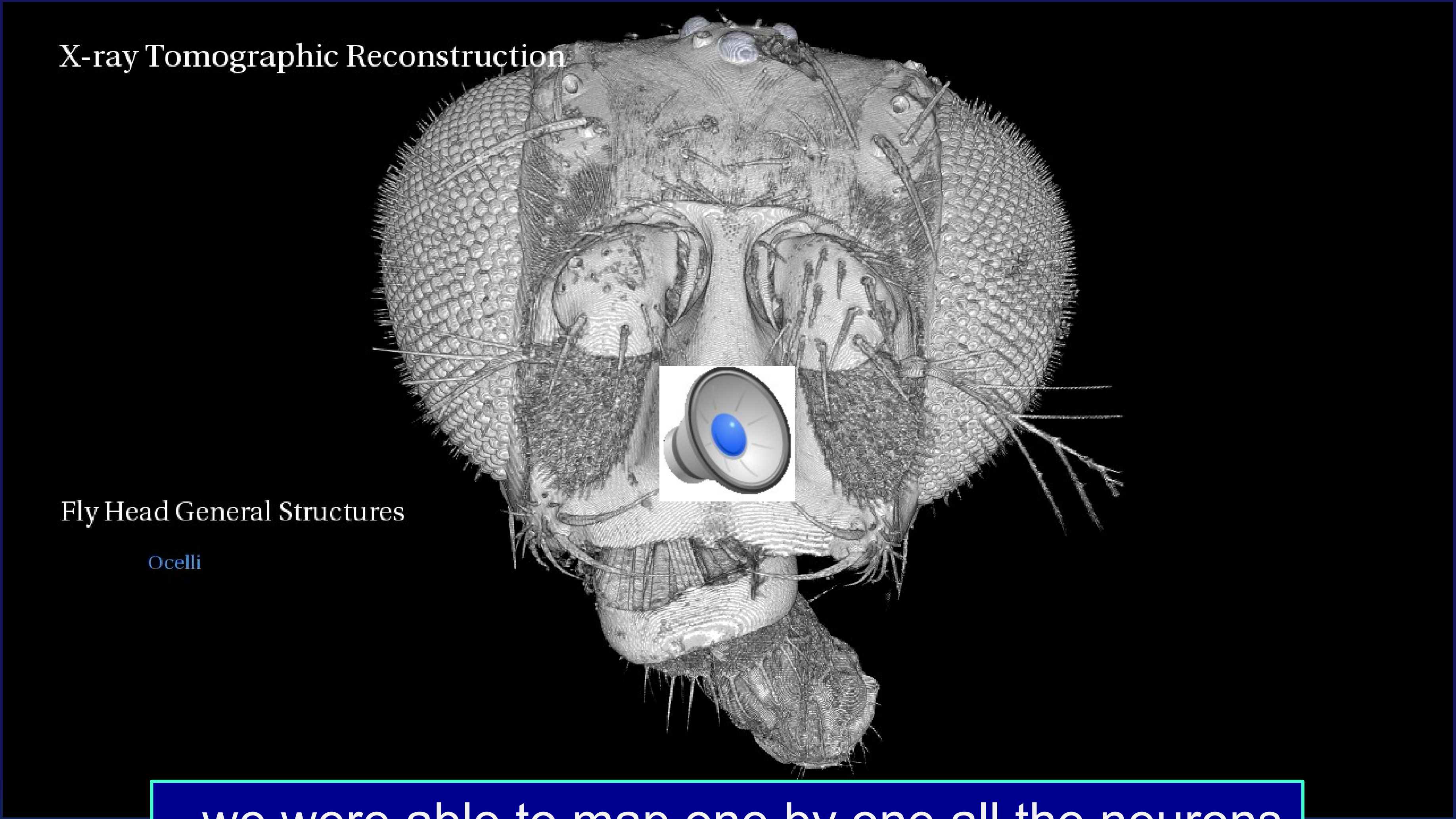
$\approx \delta^2/(\Omega D^2) \leq (\lambda D/\xi)^2/(\Omega D^2) = \boxed{\lambda^2/(\xi^2\Omega)}$ →

“coherent power factor”: if it is large, there is lateral coherence

Coherence — summary:

- Time (longitudinal) coherence requires a large coherence length $\lambda^2/\Delta\lambda$
- Spatial (lateral) coherence requires a large coherent power factor $\lambda^2/(\xi^2\Omega)$
- Due to the λ^2 terms, both are difficult to achieve for small-wavelength x-rays
- The brightness is proportional to $F/(\xi^2\Omega)$; increasing the brightness by improving the geometric parameters also increases the spatial coherence, since the conditions are the same: small ξ^2 and small Ω

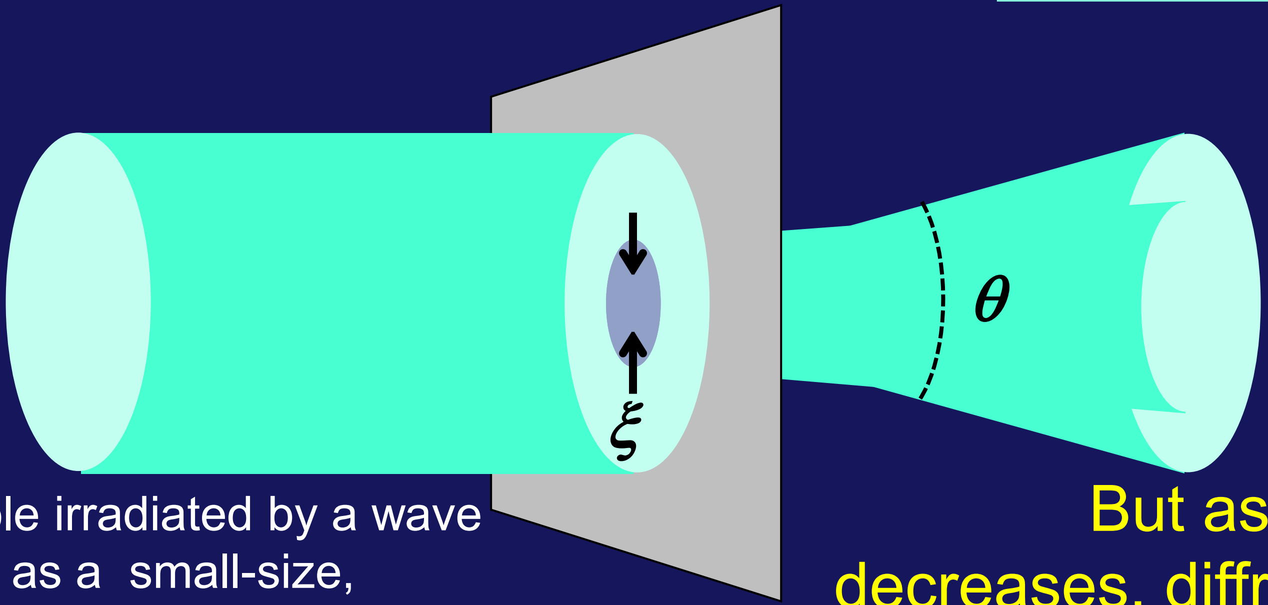
CT-scans with coherent x-rays: drosophila



we were able to map one by one all the neurons of the insect brain, and their connections!

[Y. Hwu, G. Margaritondo and A.-S. Chiang, BMC Biology **15**, 122 (2017)]

Full lateral coherence: diffraction limit



Solid
angle
$\Omega \approx \theta^2$

A pinhole irradiated by a wave can act as a small-size, spatially coherent source

But as the pinhole size decreases, diffraction increases the angular divergence

The diffraction theory gives $\xi\theta \approx \lambda$, thus $\xi^2\Omega \approx \lambda^2$

This defines the “diffraction limit” for the coherent power factor:

$$\frac{\lambda^2}{\xi^2\Omega} \approx 1$$

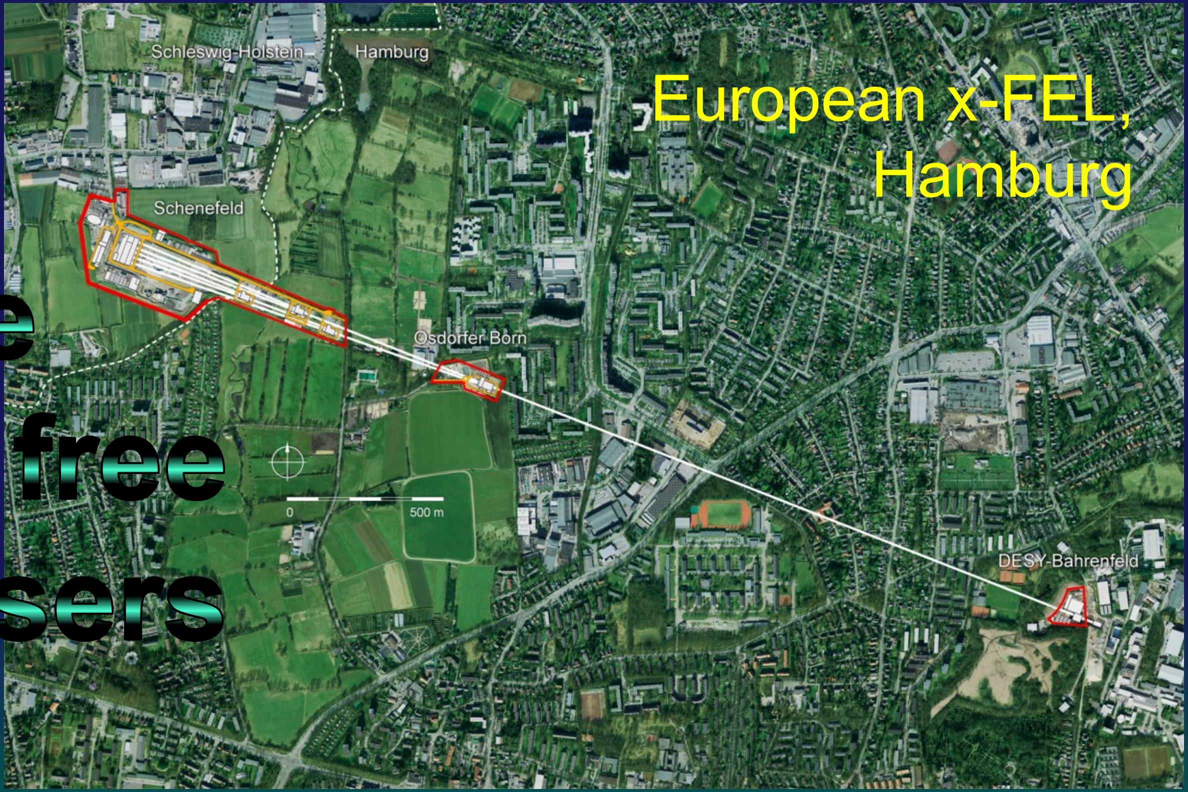
…corresponding to full spatial coherence

some synchrotrons now reach this limit – and so do x-ray FEL’s

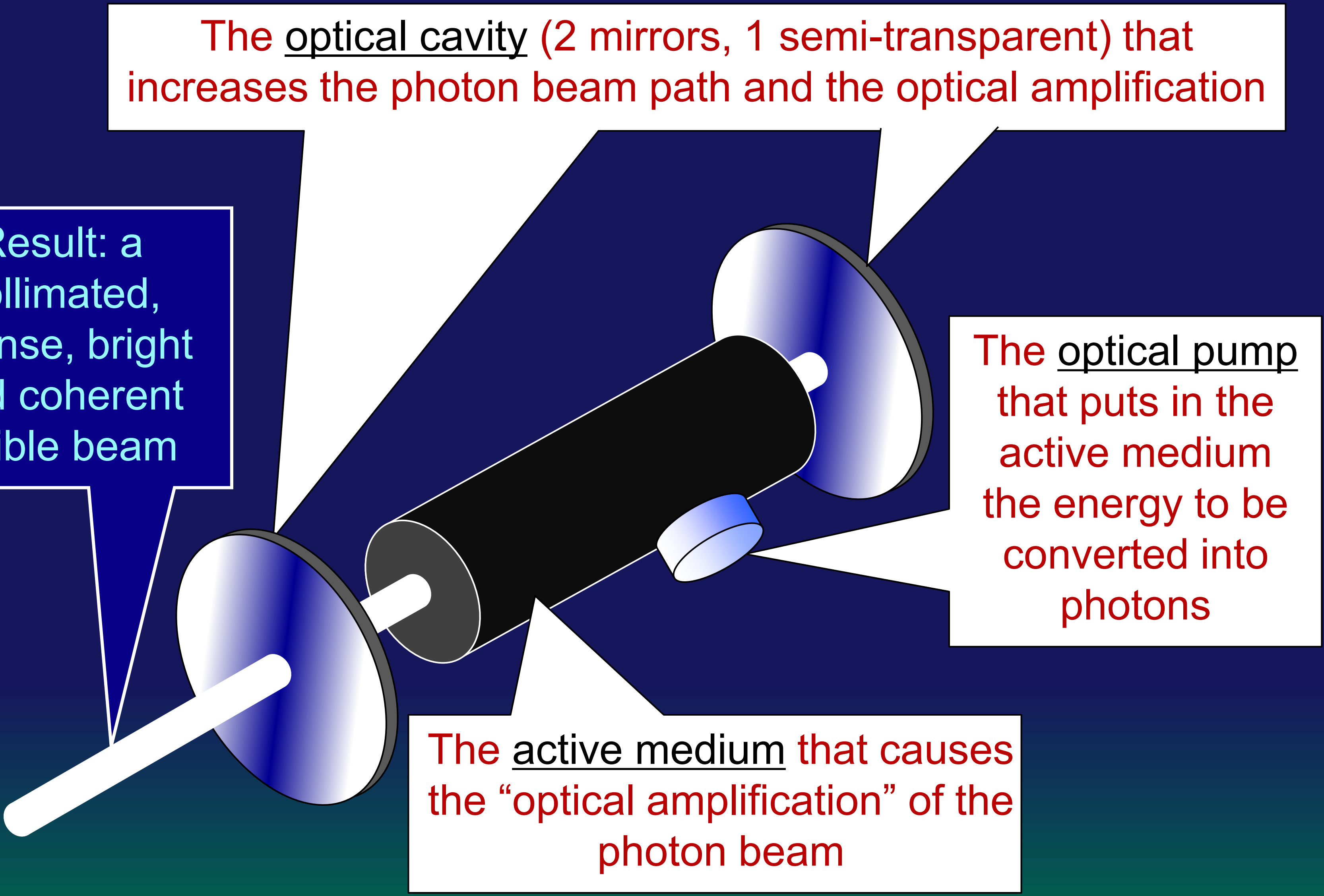
Synchrotron sources: very intense and bright, collimated, coherent, polarized:

are they lasers?

…no,
but now we have x-ray free electron lasers (x-FEL's)



To understand x-FEL's, we start from a normal laser for visible light:



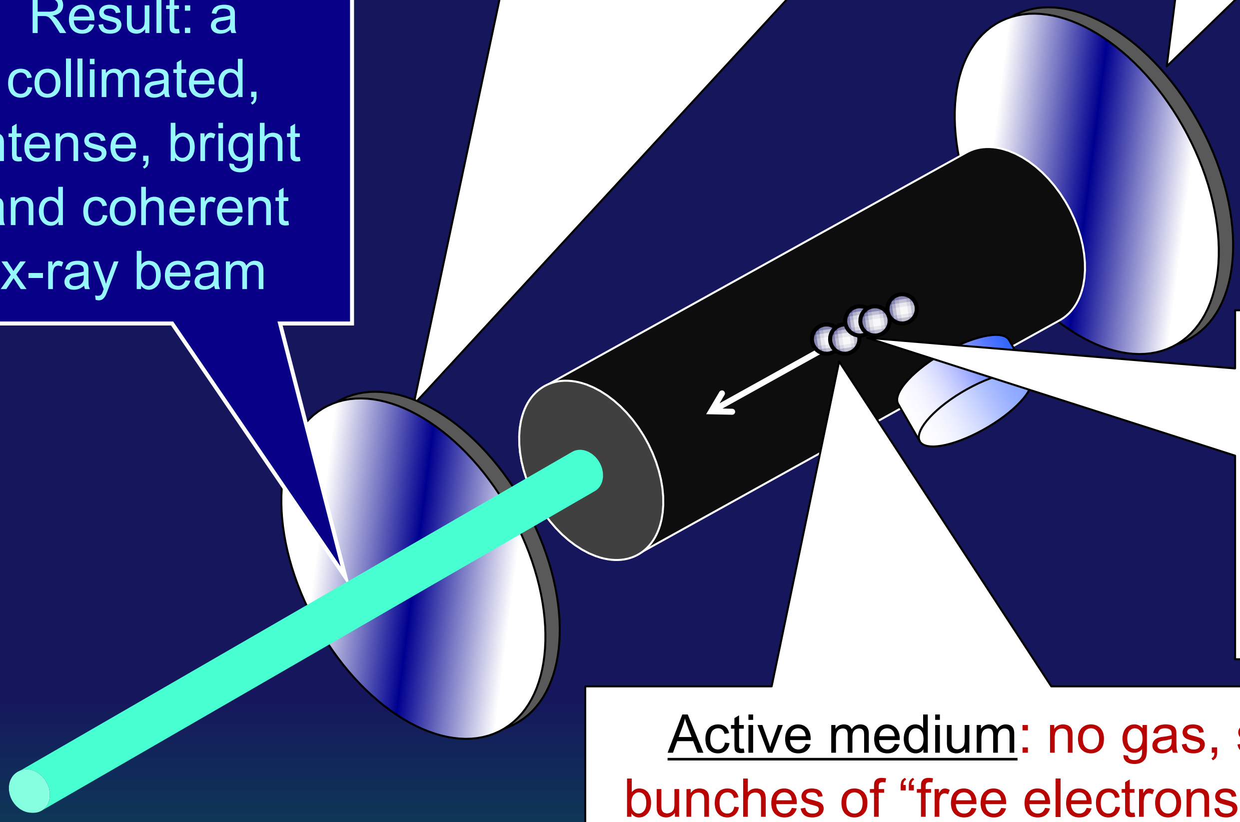
The optical cavity (2 mirrors, 1 semi-transparent) that increases the photon beam path and the optical amplification

Result: a collimated, intense, bright and coherent visible beam

The optical pump that puts in the active medium the energy to be converted into photons

The active medium that causes the "optical amplification" of the photon beam

From a normal laser to an x-FEL:



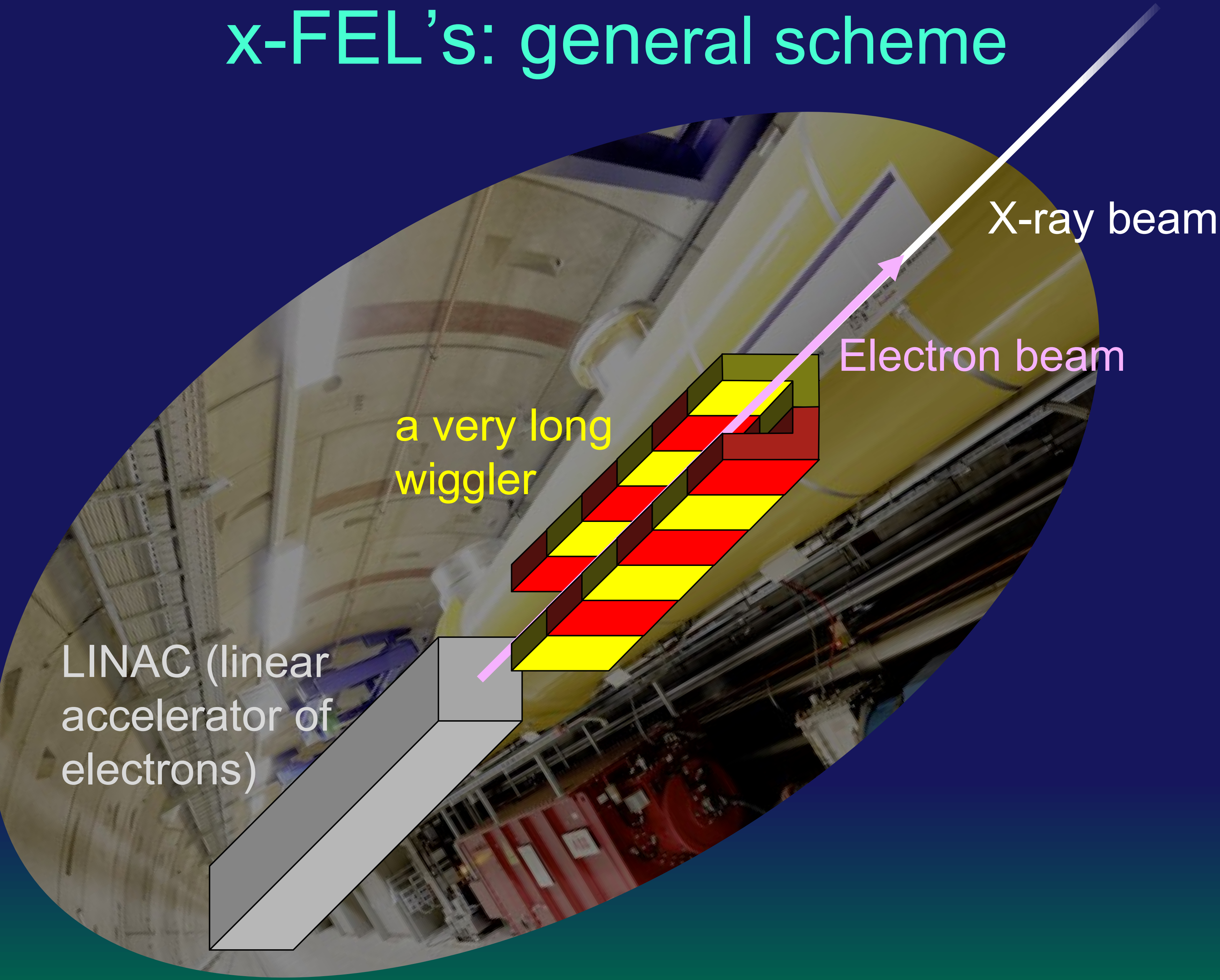
Mirrors do not reflect x-rays ⇒ no optical cavity ⇒ enough amplification needed for **one-pass lasing**

Result: a collimated, intense, bright and coherent x-ray beam

Optical pump: the free electrons themselves carry the energy and transfer it to the photons

Active medium: no gas, solid or liquid but bunches of “free electrons” in an accelerator: high power possible without damage

x-FEL's: general scheme



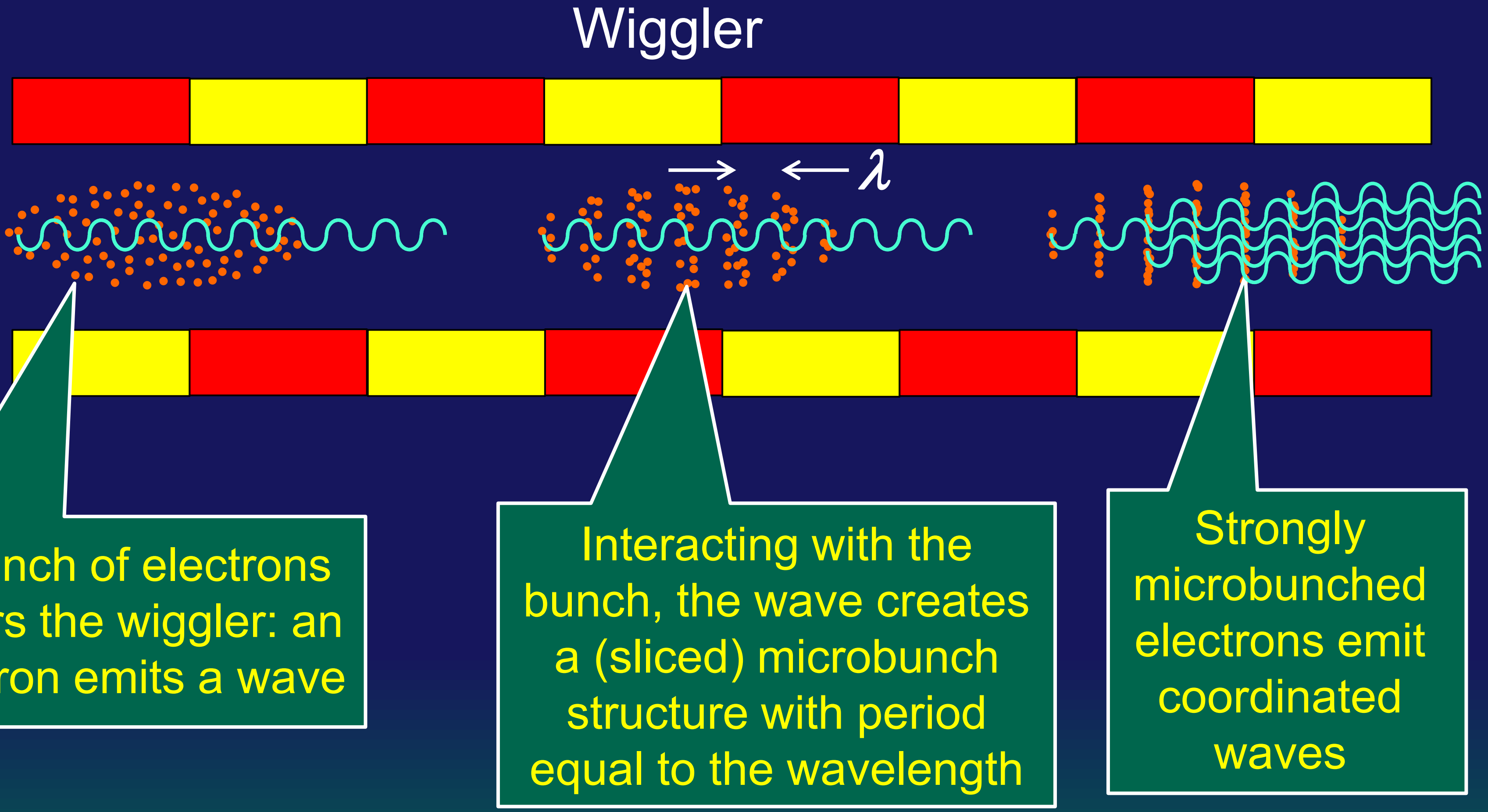
X-ray beam

Electron beam

a very long wiggler

LINAC (linear accelerator of electrons)

"sliced Italian salami": the FEL optical amplification mechanism



A bunch of electrons enters the wiggler: an electron emits a wave

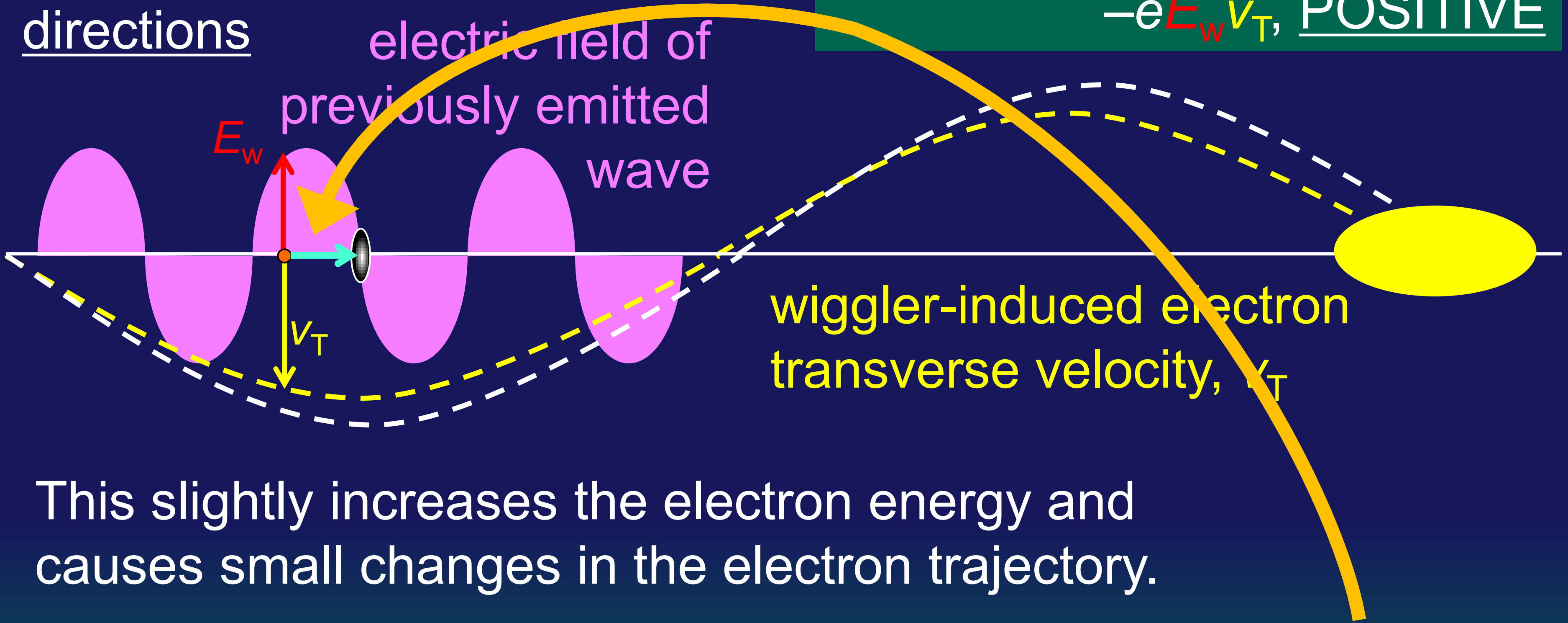
Interacting with the bunch, the wave creates a (sliced) microbunch structure with period equal to the wavelength

Strongly microbunched electrons emit coordinated waves

What causes the microbunching? (top view)

Electron charge: -*e* (negative)
Wave electric field force: $-eE_w$
Work per unit time:
$-eE_w v_T$, <u>POSITIVE</u>

Here, E_w and v_T are in <u>opposite directions</u>



electric field of previously emitted wave

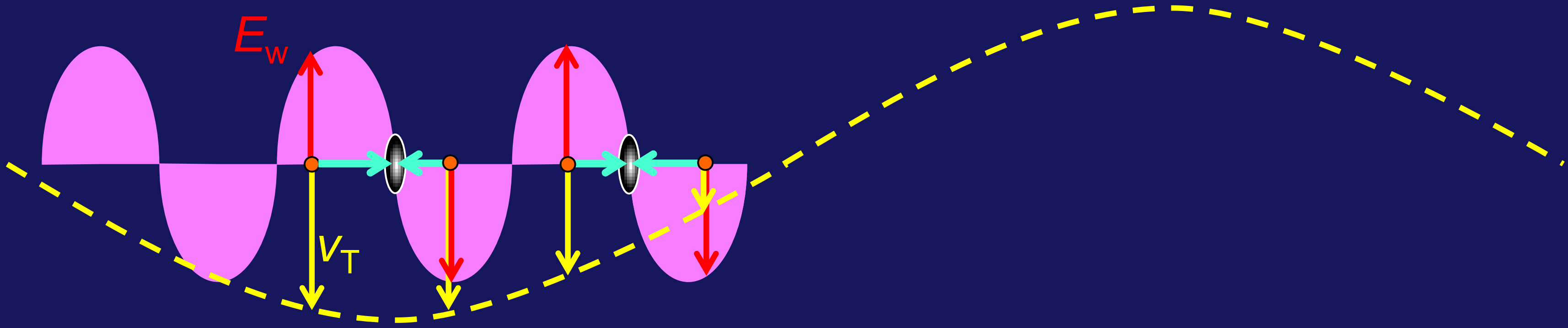
wiggler-induced electron transverse velocity, v_T

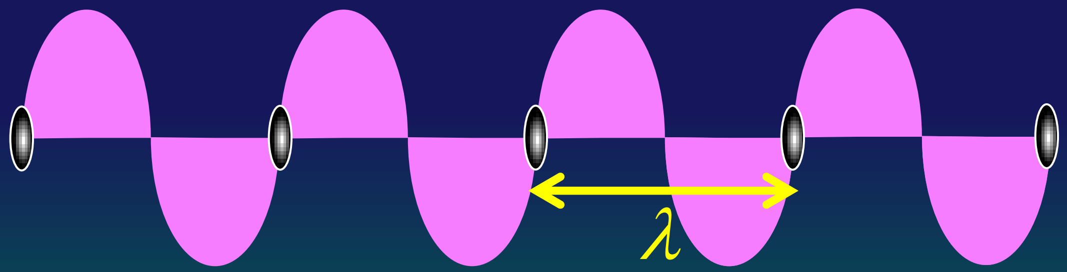
This slightly increases the electron energy and causes small changes in the electron trajectory.

Longitudinally, the effect is equivalent to a force that "pushes forward" the electron towards a wave node

What happens to other electrons?

Look at the directions of E_w and v_T: the electrons are pushed towards every other wave node

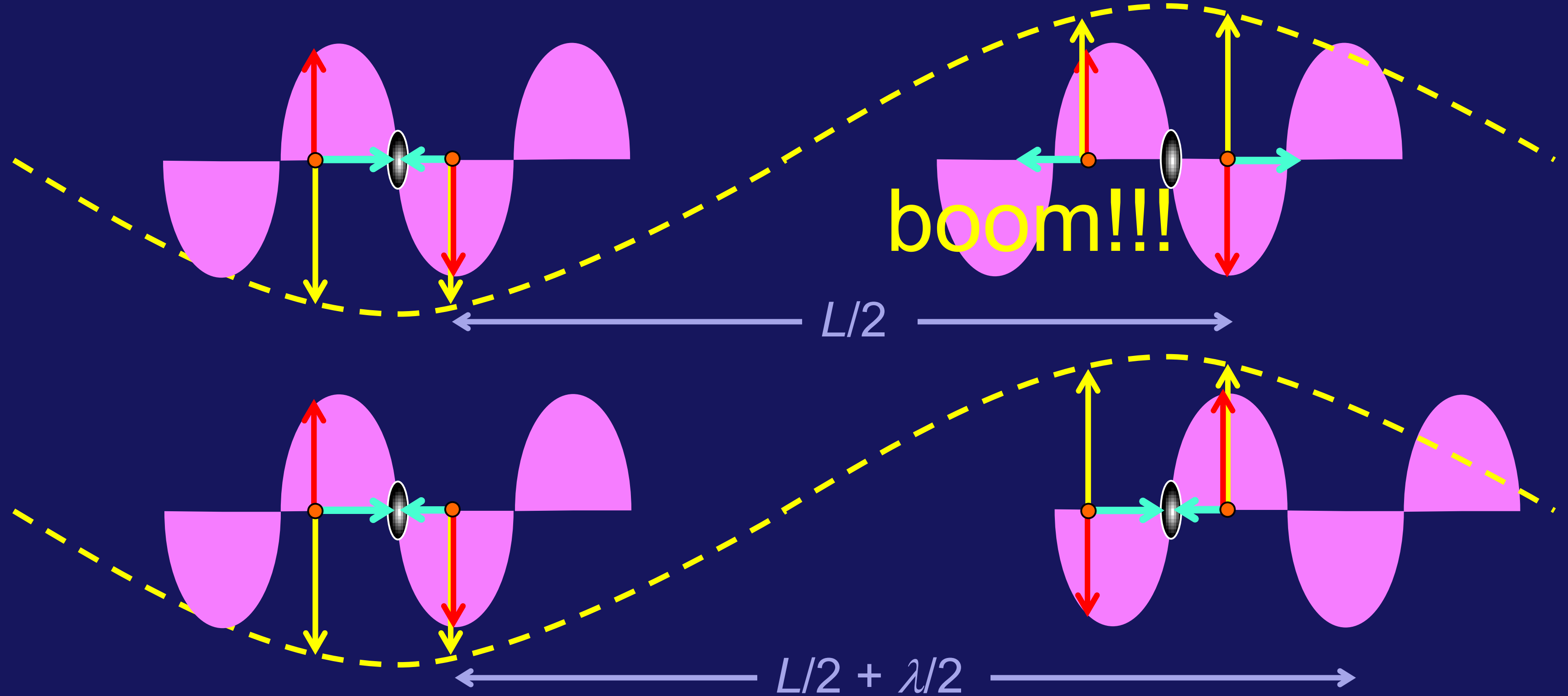




This creates the microbunches, with period equal to the wavelength

However, something seems wrong…

…if the electrons and the wave travel together, after one-half wiggler period the vectors E_w should be the same but the transverse velocities and the pushing directions should be reversed, destroying the microbunches

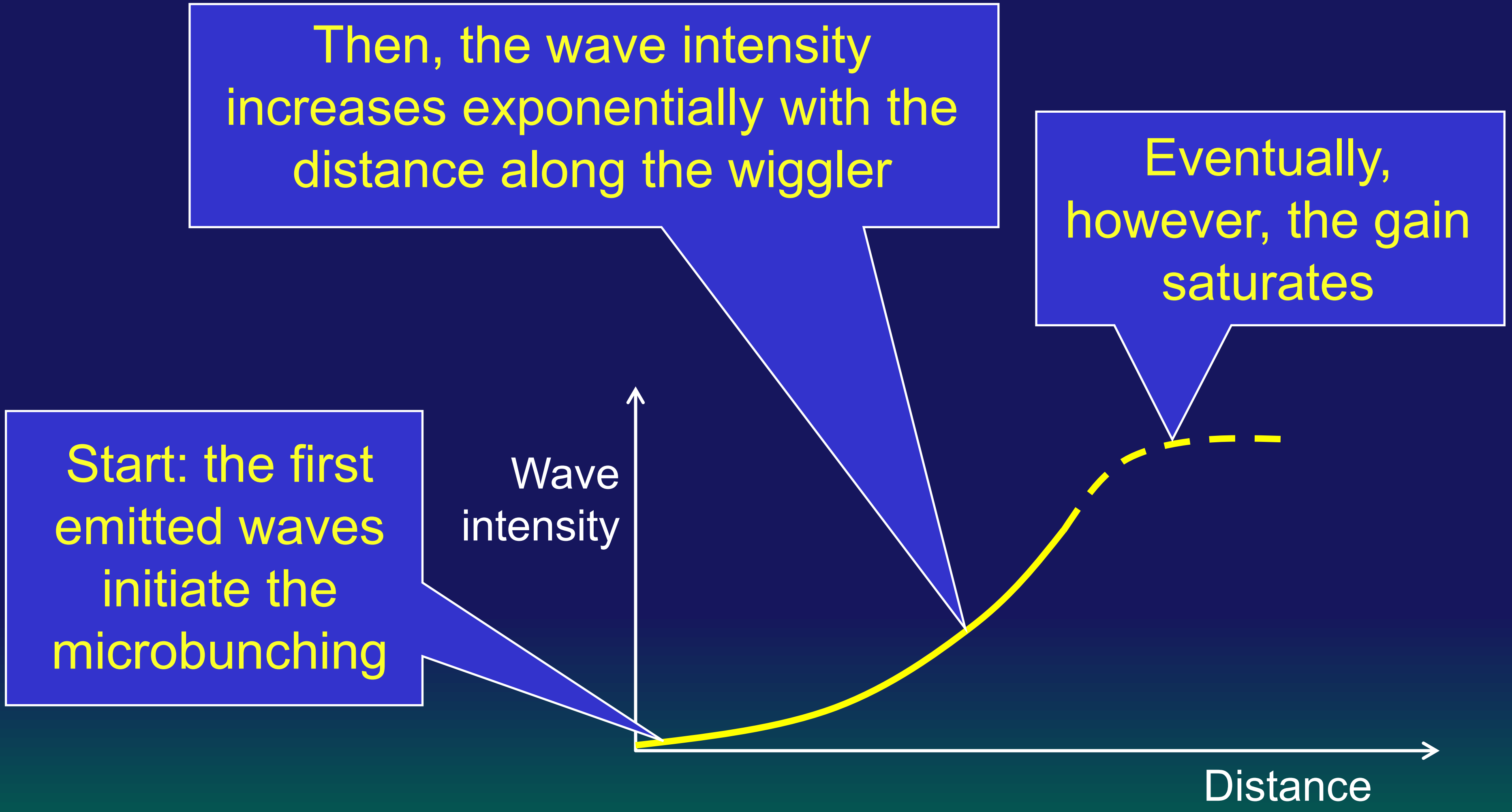


IS THIS TRUE? NO!

The electrons do not travel with the wave but a different speeds $v \neq c$. As they travel over $L/2$, the wave path is $c(L/2)/v$. The path difference is $(L/2)(c/v - 1) = (L/2)(c/v)(1 - v/c\ ) = (L/2)(c/v)((1 - v^2/c^2)/(1 + v/c) \approx L/(4\gamma^2) = \lambda/2$

…just right for microbunching to continue: FEL’s are a MIRACLE!

Microbunching and coordinated emission produce a progressive increase of the wave (Self-Amplified Spontaneous Emission, SASE)



Then, the wave intensity increases exponentially with the distance along the wiggler

Eventually, however, the gain saturates

Start: the first emitted waves initiate the microbunching

What causes the exponential intensity increase along the wiggler?

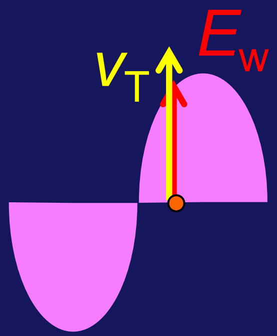
- Define: I = wave intensity; E_w = wave E-field, proportional to $\sqrt{I}$
- v_T = electron transverse velocity
- dI /dt = energy transfer rate (electrons→wave), determined by: (1) the transfer rate for one electron, (2) the microbunching
- The one-electron transfer rate is given by the (negative) work, proportional to $E_w v_T$
- The microbunching is proportional to E_w

- **dI /dt is proportional to $E_w E_w$ and therefore to $\sqrt{I}\,\sqrt{I} = I$**
- **dI /dt = C I , with C = constant corresponds to $I = I_o\exp(Ct)$, an exponential increase of I with t , and also with the distance = vt**

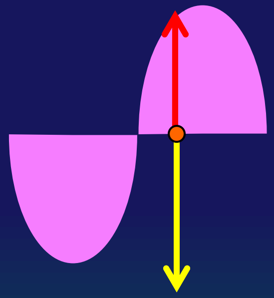
Why does the intensity increase saturate?

After a certain distance, the microbunching is complete, and the amplification slows down

Plus, the electrons lose energy to the wave and their γ decreases, changing the emitted wavelength $L/(2\gamma^2)$: they no longer contribute to the wave intensity



Also note: for electron→wave energy transfer, the directions of v_T and of the wave E-field must produce negative work: this is true here



But, as the electron gives energy to the wave, it slows down: the direction of v_T relative to E_w changes.

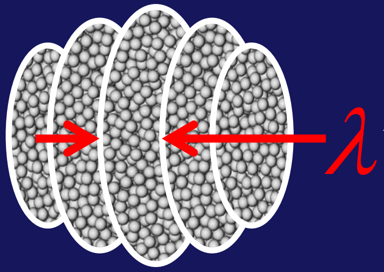
Eventually, this leads to wave → electron energy transfer

The electrons accelerate until they reach again the conditions for electron → wave energy transfer

The mechanism goes on and on, with electrons-wave energy oscillations rather than a continuous wave amplification

Another paradox?

At short wavelengths, free electron lasing is very difficult : x-FEL's were realized only several decades after the infrared FEL's

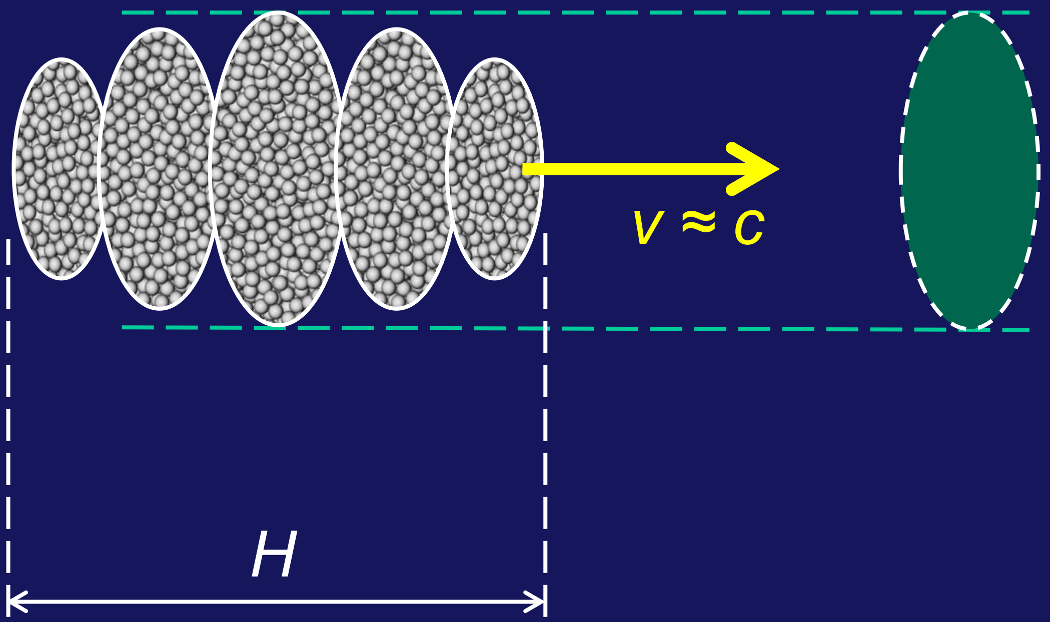


…but why? At short x-ray wavelengths the microbunches are close to each other and require short shifts of the electrons inside their bunches: should microbunching be easier?

NO, BECAUSE:

- A short wavelength $L/(2\gamma^2)$ requires a large γ
- A large γ boosts the longitudinal relativistic mass $\gamma^3 m_o$, making the electrons "heavy" and difficult to move to the microbunches
- Furthermore, the small spacing between microbunches makes the microbunched structure very vulnerable to perturbations
- Finally, one-pass lasing requires, besides a long wiggler, a very small, high-density electron bunch, i.e., an excellent electron beam control (this is why "normal" wigglers are not x-FEL's)

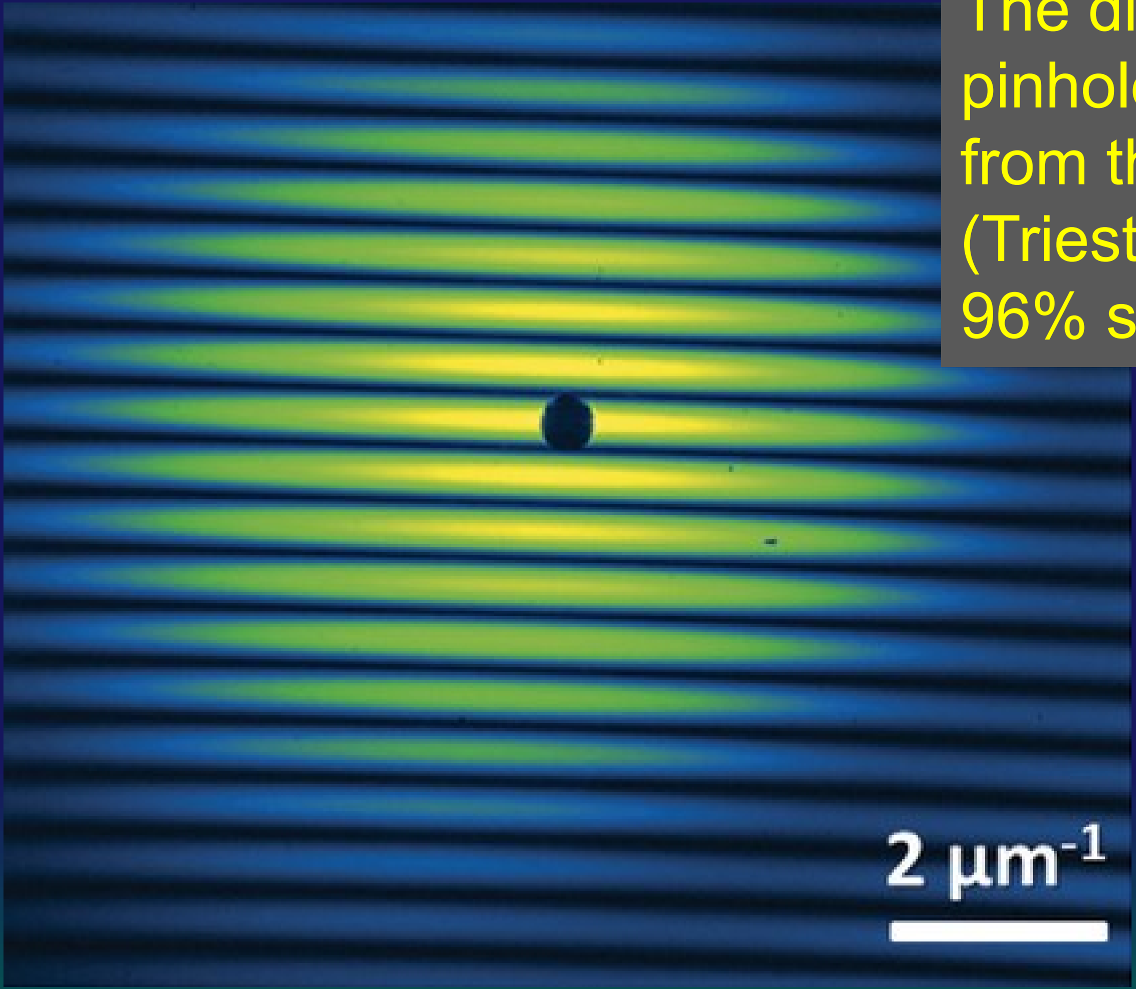
Geometry and duration of an FEL pulse:



One-pass lasing requires a very small electron bunch cross section, producing a small transverse size of the photon pulse

Likewise, the electron bunch length H must also be very small, corresponding to a small photon pulse duration $H/v \approx H/c$, in the femtosecond range or less

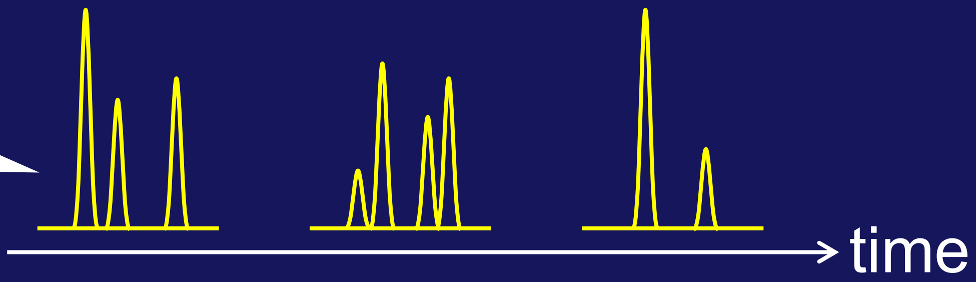
The spatial coherence of x-FEL's is high (close to the diffraction limit)



The diffraction by two pinholes of 32.5 nm pulses from the FERMI FEL (Trieste) demonstrates 96% spatial coherence

On the contrary, a serious problem affects the x-FEL time (longitudinal) coherence:

SASE amplifies waves that are stochastically emitted when the electron bunch enters the wiggler



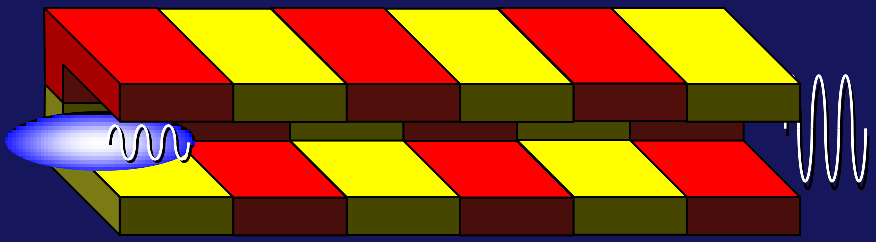
The time structure changes from pulse to pulse, broadening the wavelength spectrum and limiting the time coherence

Possible solution: “seeding”, i.e., amplifying a wave with high time coherence, produced by an external source and injected into the x-FEL

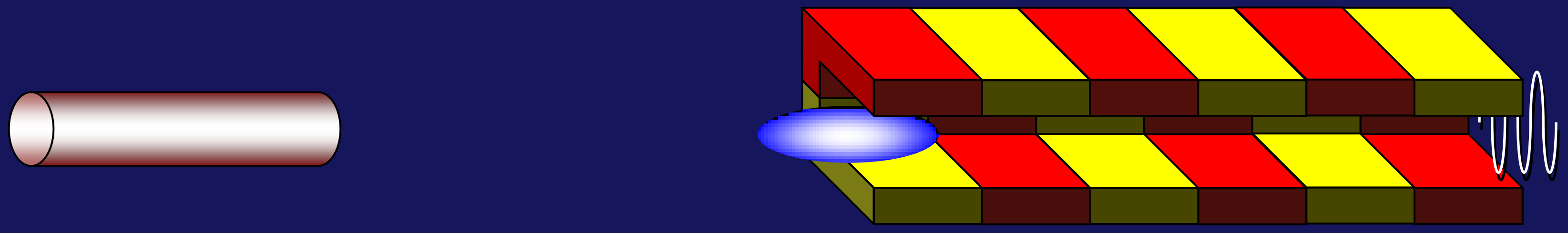
A complicated technology, but now a reality

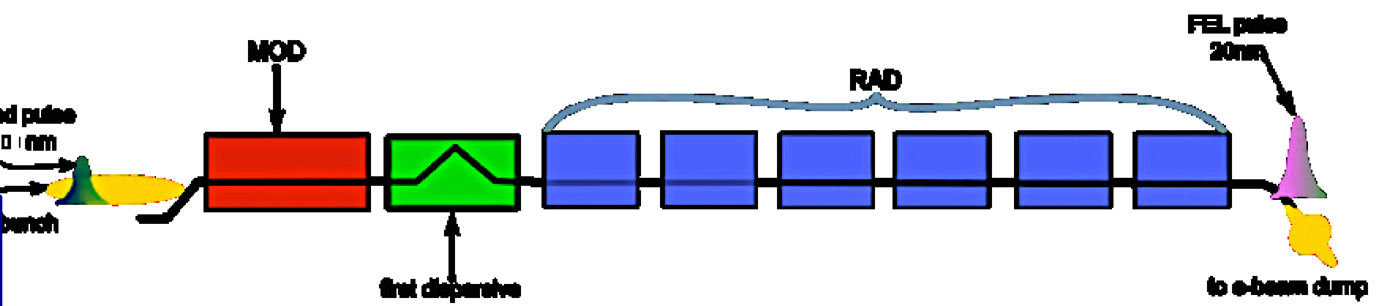
SASE vs. seeding:

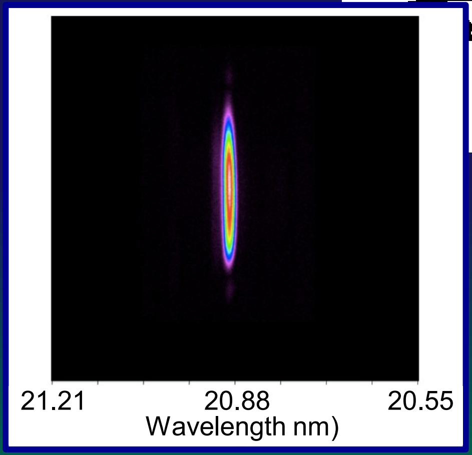
SASE amplifies waves spontaneously (randomly) emitted by electrons as the bunch enters the wiggler



Seeding amplifies waves injected by an external source



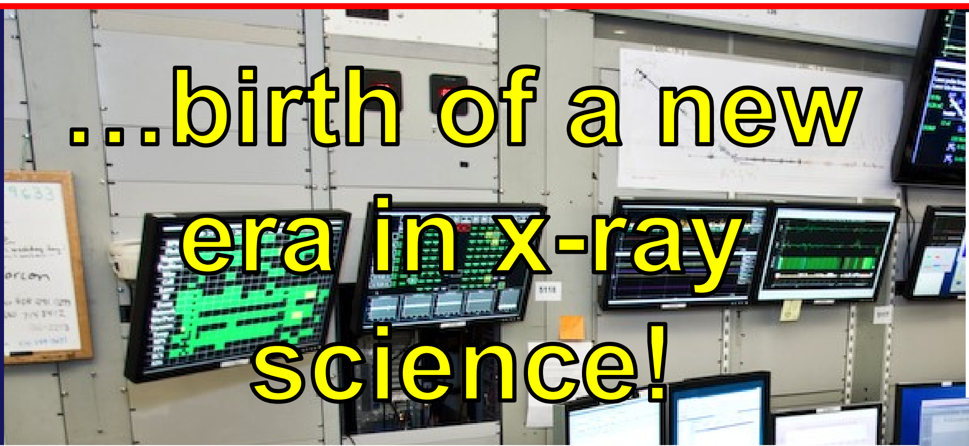




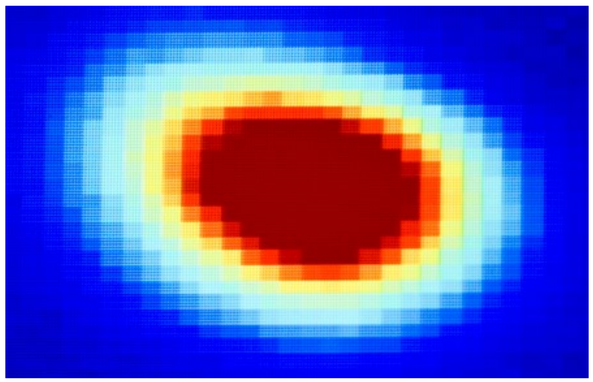
The seeded x-FEL FERMI (Trieste): the narrow wavelength bandwidth demonstrates high time coherence (E. Allaria et al., Nature Photonics **6**, 699 (2012) and **7**, 913 (2013)

April 21, 2009 New Era of Research Begins as World's First Hard X-ray Laser Achieves First Light

X-ray laser pulses of unprecedented energy and brilliance produced at SLAC



...birth of a new era in x-ray science!



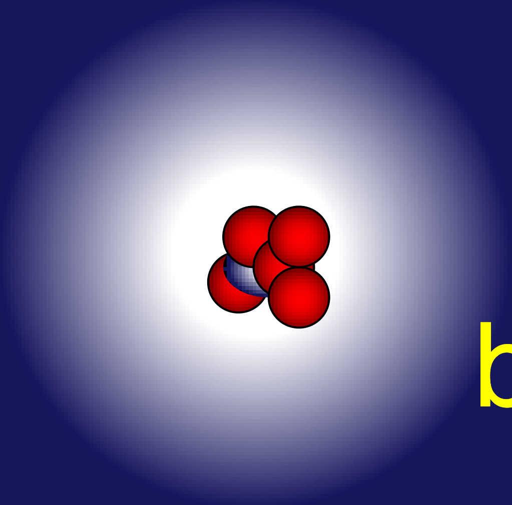
Claudio Pellegrini, UCLA -- father of the x-FEL theory

The European x-FEL in Hamburg

X-ray FEL’s are now a reality:
what can we do with them?

x-FEL’s emit femtosecond pulses of tens of gigawatts: <u>how</u> can we handle all this power, and how can we use it?

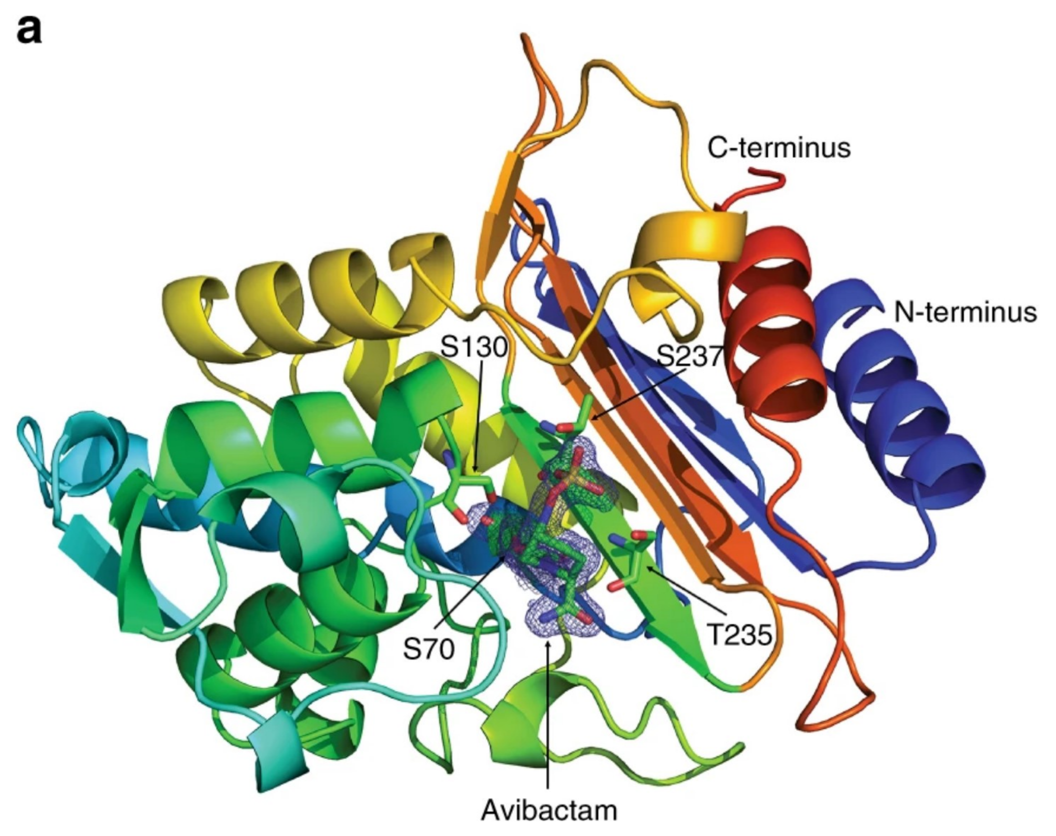
…sent into a molecule or a nanoparticle, it causes an explosion:



boom!

…but, as the pulse is ultrashort, we can try to extrapolate from diffraction data the structure <u>before</u> the explosion

A nice case of structure determination from serial one-shot data at the European X-FEL



Structure of CTS-M-14 β-lactamase, a previously unknown complex involved in antibiotic resistance [M. O. Wiedorn, D. Oberthür and A. Barty, Nature Communications **9**, 4025 (2018)]

What happens at the femtosecond scale?

Fast chemical reactions

In 100 femtoseconds shock and sound waves travel in solids over atomic distances

A water molecule dissociates in 10 femtoseconds

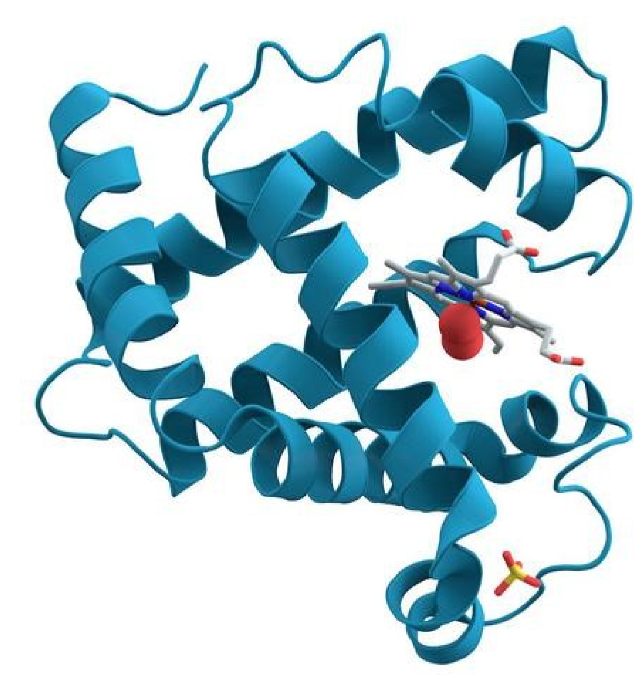
Photons propagate over hundreds of nanometers

Typical periods of molecular vibrations: 10-100 femtoseconds

Laser surgery without collateral damage

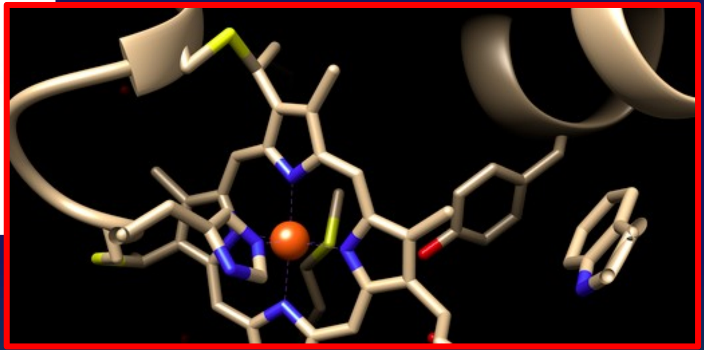
Novel micromachining techniques, etc…

Using ultrafast x-FEL pulses to find the time-dependent structures of the nitrosyl-myoglobin and cytochrome *c* proteins at the European x-FEL – essential to understand how our body works



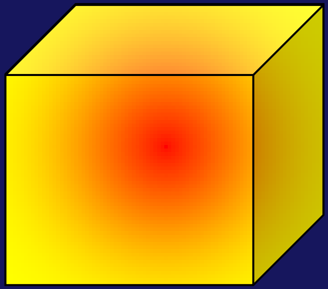
First step: using an optical laser pulse to trigger detachment of a molecule or an electronic transfer

Second step: using an ultrashort x-FEL pulse to find the time-dependent structure of the evolving molecule



[D. Kinschel et al., Nature Communications 11, 4145 (2020);
C. Bacellar et al., PNAS 117, 21914 (2020)]

The high power and energy density of an x-FEL can create extreme short-lived conditions for materials



HED (High Energy Density) regime:

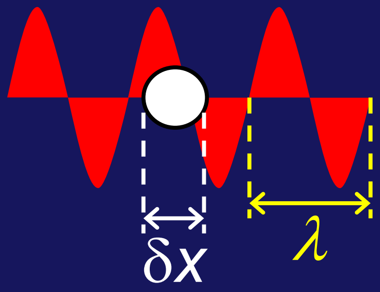
- Extreme pressure
- Extreme temperature
- Extreme density, etc…

The experiments are important for:

- Nuclear fusion research
- Laboratory astrophysics
- Technology of high-power sources, and other fields

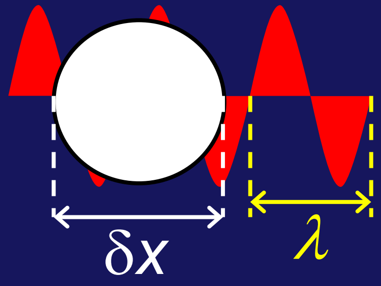
Novel x-FEL applications: exploiting coherence as a quantum property

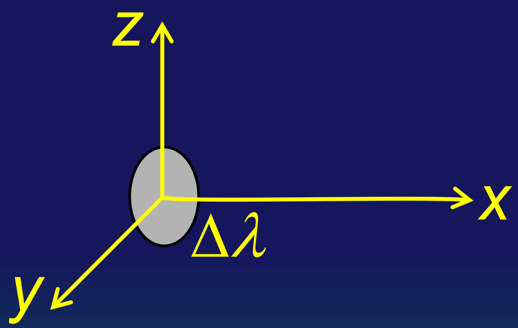
In quantum electrodynamics (QED), the radiation consists of particles (photons): can they cause wave-like interference and diffraction?



NO – if the “size” of each photon is smaller than one wavelength

YES – if the photon size is bigger than one wavelength





Photon “size” in the longitudinal *x*-direction = Heisenberg uncertainty: $\delta x \approx \hbar / \delta p_x$

$p_x \approx p = \hbar / \lambda$; $\delta p_x \approx (dp / d\lambda)\Delta\lambda = \hbar\Delta\lambda / \lambda^2$

$\delta x \approx \lambda^2 / \Delta\lambda = L_c$, the “coherence length”

…we thus re-discover the condition for wave-like phenomena: $L_c > \lambda$, thus $\Delta\lambda/\lambda < 1$

The links between coherence and quantum electrodynamics are very deep – see a very nice recent article by Joachim Stöhr [Synchrotron Radiation News 32 (2019)]

I will outline in simple terms how the wave picture of light does in fact emerge from QED in lowest (first) order, why in the past there has been no need to develop a quantum theory of X-ray diffraction, and why with the advent of XFELs this is changing

First-order QED: (1) interference and diffraction are only wave-like interactions of each photon with itself. (2) Multiple-photon effects are negligible.

BUT: with “seeded” x-FELs point (2) can change and lead to new techniques.

…look at the next talk of this conference, by Paris Tzallas

At the end of our journey, I would like to thank:

- Primoz Rebernik for his key contributions to our FEL theory
- Maya Kiskinova, Yeukuang Hwu and their coworkers for disclosing important experimental results
- The Science@FELs 2020 organizers for their kind invitation

...and thanks
for the attention:
your future, young folks,
looks brighter than ever!