X-ray free electron lasers

F. Grüner (LMU+MPQ), July 15, 2005, Photonics Lecture, Prof. Krausz

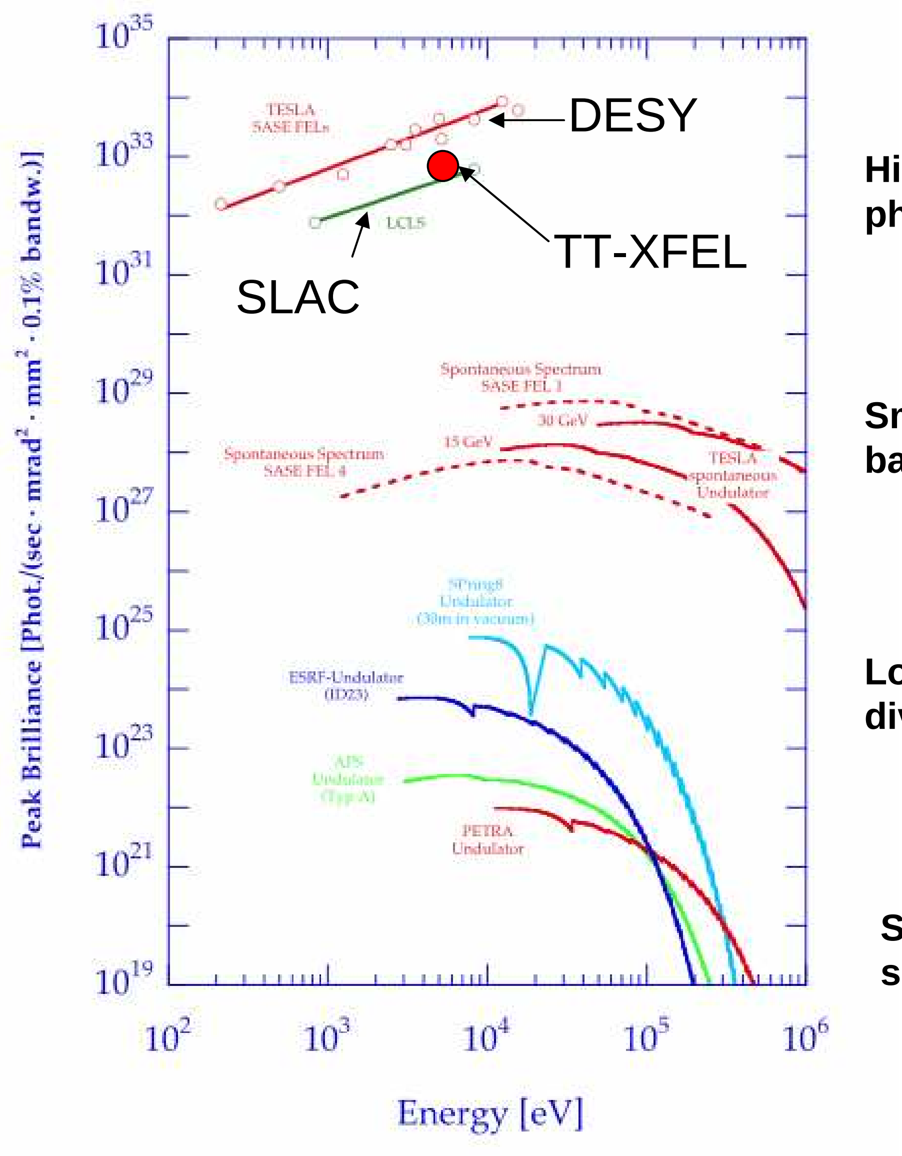
- Motivation for FELs
- What is an FEL?
- Undulators and Wigglers
- SASE and X-Ray-FEL (XFEL)
- Bubble-XFEL

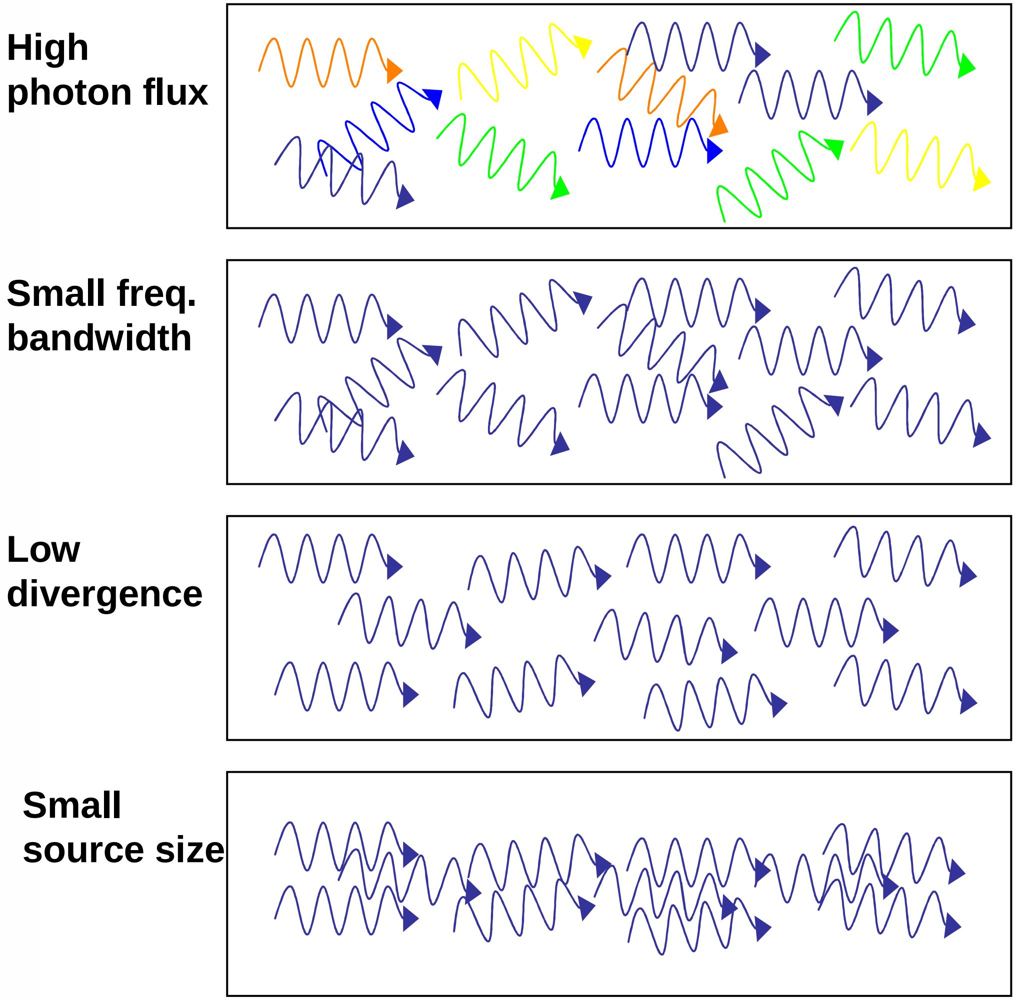
Motivation for Photons

- why trying to “transform” bubble **electrons** into **photons**?
- advantage of photons:
  - photons as **atomic probes** both in *space* and *time*
    - energy of 15 keV corresponds to wavelength of 0.8 Å
    - pulses can be on scale of attoseconds (1 as = 10^{-18} s)
    - atomic scale of space = a_0 = 0.53 Å (Bohr radius)
    - atomic scale of time ≈ $2\pi a_0/v_0$ ≈ 150 as ($v_0 \approx c/137$)
  - X-ray photons can penetrate matter well beyond surface
  - (**ultrabrilliant**) photons can image a *single* molecule

FEL as a High-Brilliance Light Source

[Peak brilliance] = Photons/(s·mrad²·mm²·0.1%bandwidth)





Why an X-ray Free-Electron Laser ?

- time scale of chemical reactions: fs
- X-ray: wavelength of atomic scale
- fs-X-ray pulse → “4D imaging with atomic resolution”

- ultrafast chemistry & biology:
  - ❑ conformational changes
  - ❑ electron transfers in molecules
- phase transitions in material science
- inner shell ionization

- **single molecule imaging**

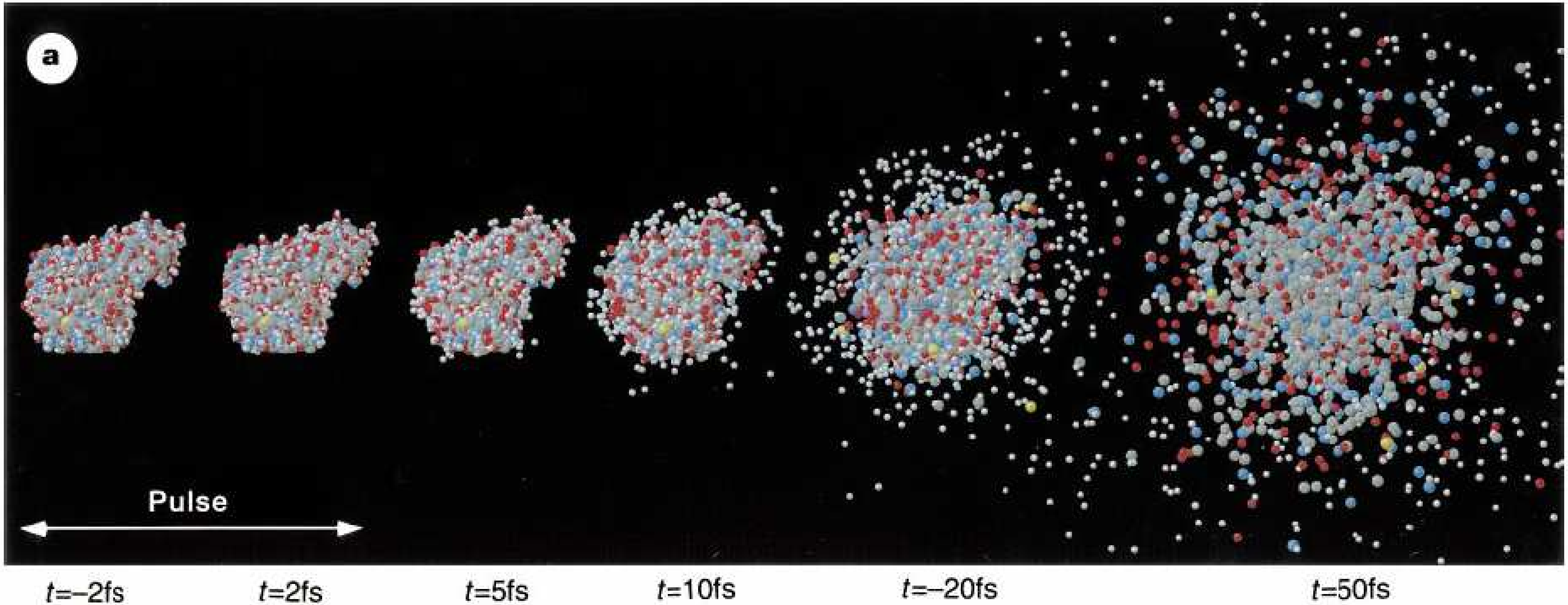
Single Molecule Imaging I

• why ***single*** molecule imaging?

→ 70 % of all proteins in medical drugs cannot be **crystallized**!

• problem: Coulomb explosion

→ ***ultrafast*** X-ray pulses needed:



Single Molecule Imaging II

- how to extract **structure** information?

change in wave vector due to scattering

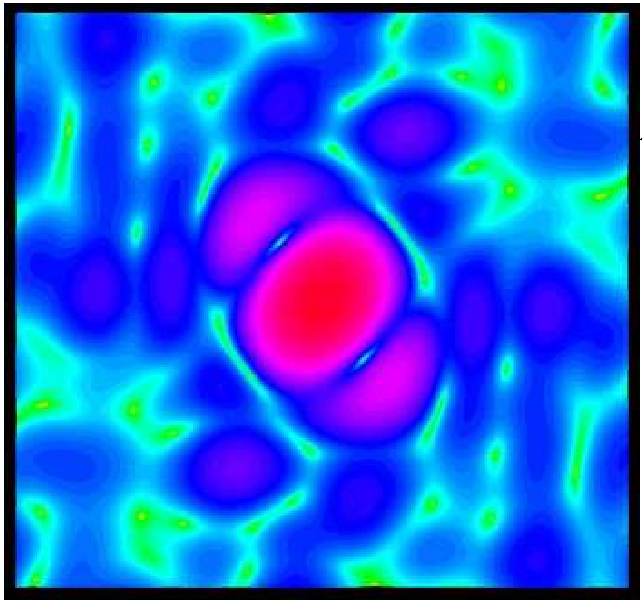
$$I(\mathbf{u},\Omega) = 1/2(1+\cos^2 2\theta)\Omega r_e{}^2 \int_{-\infty}^{\infty} \mathrm{I}(\mathrm{t}) \left| \sum_j f_j(\mathrm{t})\exp\{\mathrm{i}\Delta\mathbf{k}(\mathbf{u})\cdot\mathbf{x}_j(\mathrm{t})\} \right|^2 \mathrm{dt}$$

mean **number** of elastically scattered **photons** into pixel of a CCD

intensity of X-ray pulse

form factor of j-th atom

Time-dependent **position** of atoms in molecule (Coulomb explosion!)

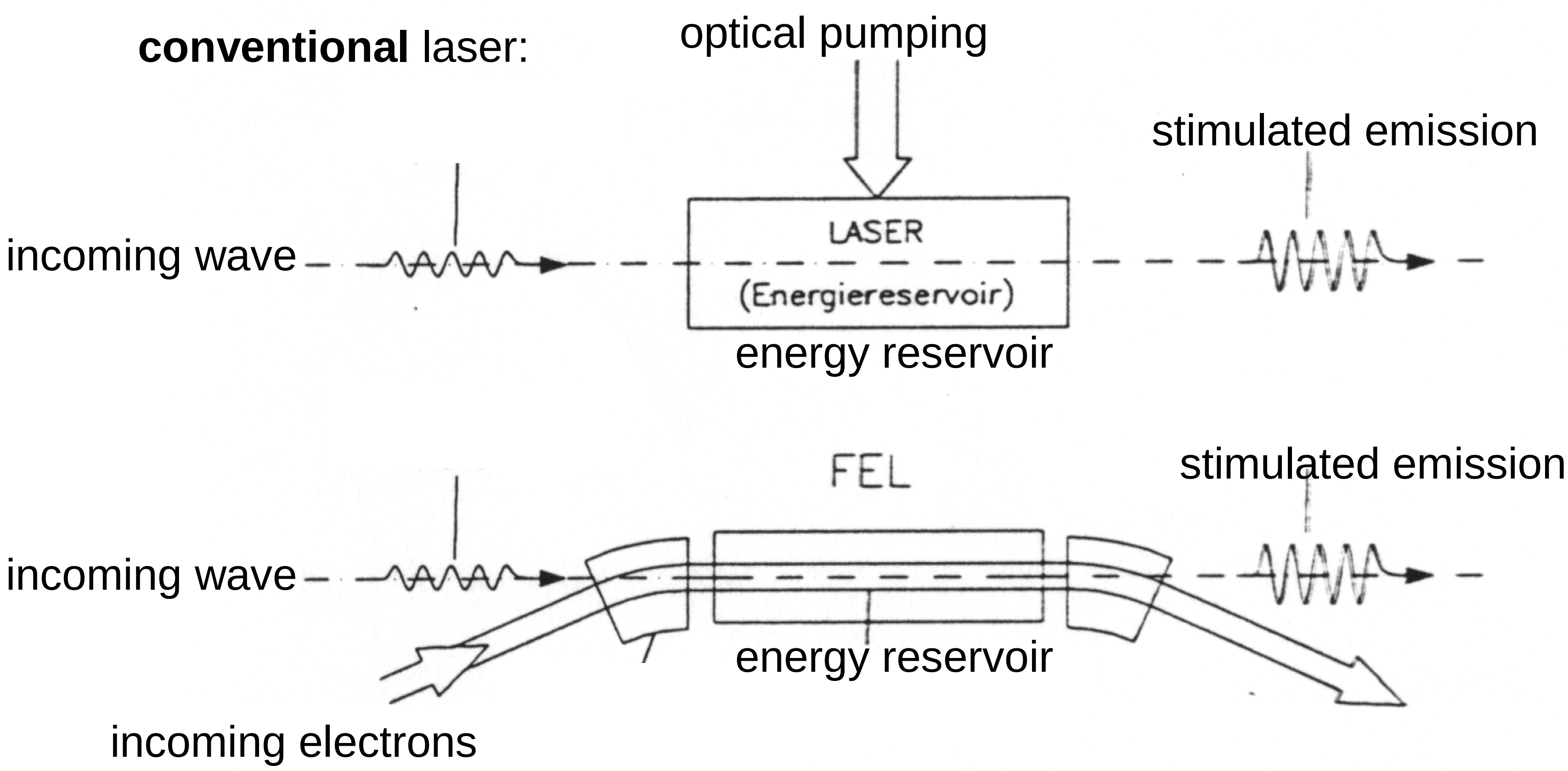


diffraction pattern of **single** shot

- ~1000 single shots necessary
- for each shot extract orientation
- superpose all shots
- extract structure information

What is a Free-Electron Laser ?

- **FEL** = **F**ree-**E**lectron **L**aser



- **SASE** = **S**elf-**A**mplification of **S**pontaneous **E**mission:

thus, no seeding field required → XFEL realizable

Spontaneous Synchrotron Radiation:

Power

non-relativistic:

$$P = \frac{e^2}{6\pi\varepsilon_0 m_0^2 c^3}\left(\frac{d\vec{p}}{dt}\right)^2$$ ← *momentum*

relativistic:

$$dt \rightarrow d\tau = \frac{1}{\gamma} dt \qquad \left(\frac{dp_\mu}{d\tau}\right)^2 \rightarrow \left(\frac{d\vec{p}}{d\tau}\right)^2 - \frac{1}{c^2}\left(\frac{dE}{d\tau}\right)^2$$

$$P = \frac{e^2}{6\pi\varepsilon_0 m_0^2 c^3}\left(\left(\frac{d\vec{p}}{d\tau}\right)^2 - \frac{1}{c^2}\left(\frac{dE}{d\tau}\right)^2\right)$$

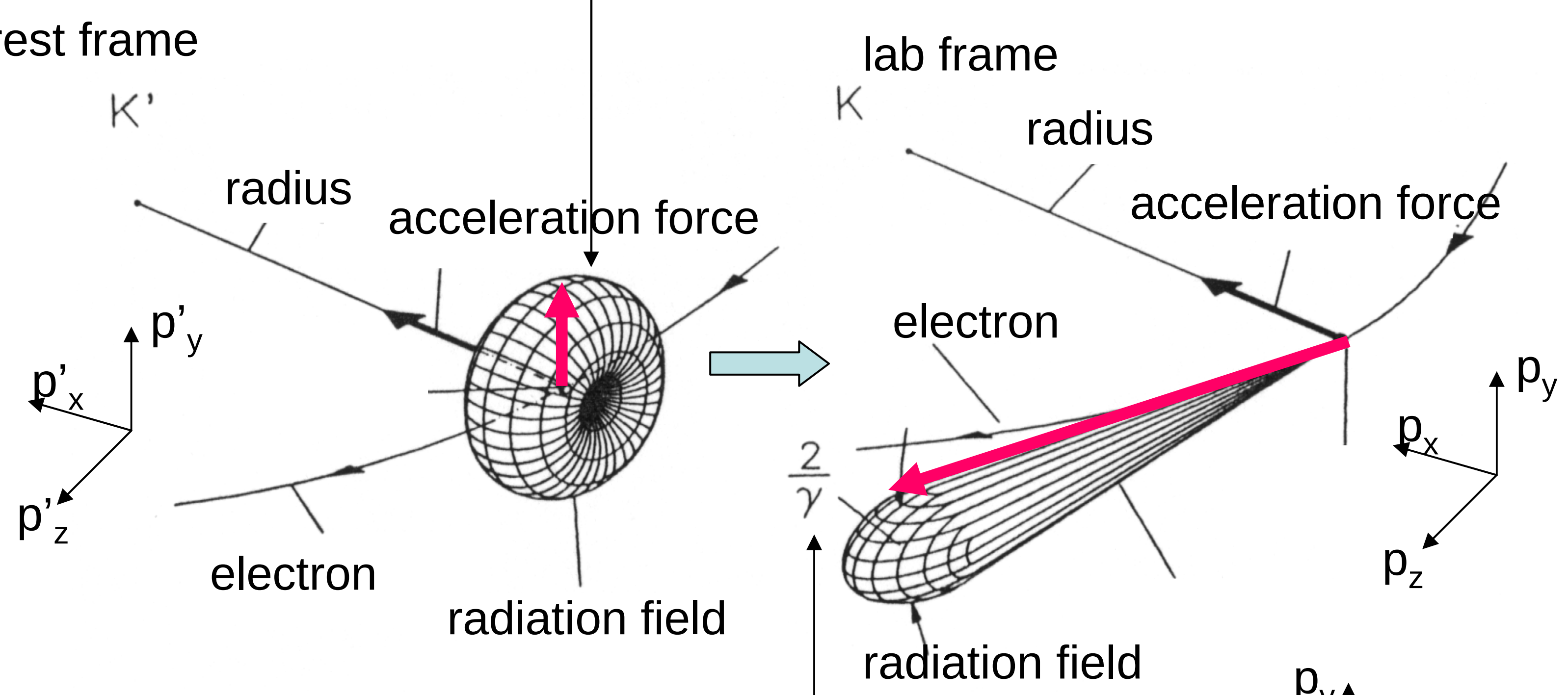
magnetic deflection: $\frac{dE}{d\tau} = 0$

$$P = \frac{e^2}{6\pi\varepsilon_0 m_0^2 c^3}\left(\left(\frac{d\vec{p}}{d\tau}\right)^2\right) = \frac{e^2\gamma^2}{6\pi\varepsilon_0 m_0^2 c^3}\left(\frac{d\vec{p}}{dt}\right)^2$$

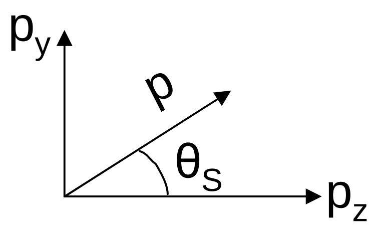
Spontaneous Synchrotron Radiation:

Emission Angle

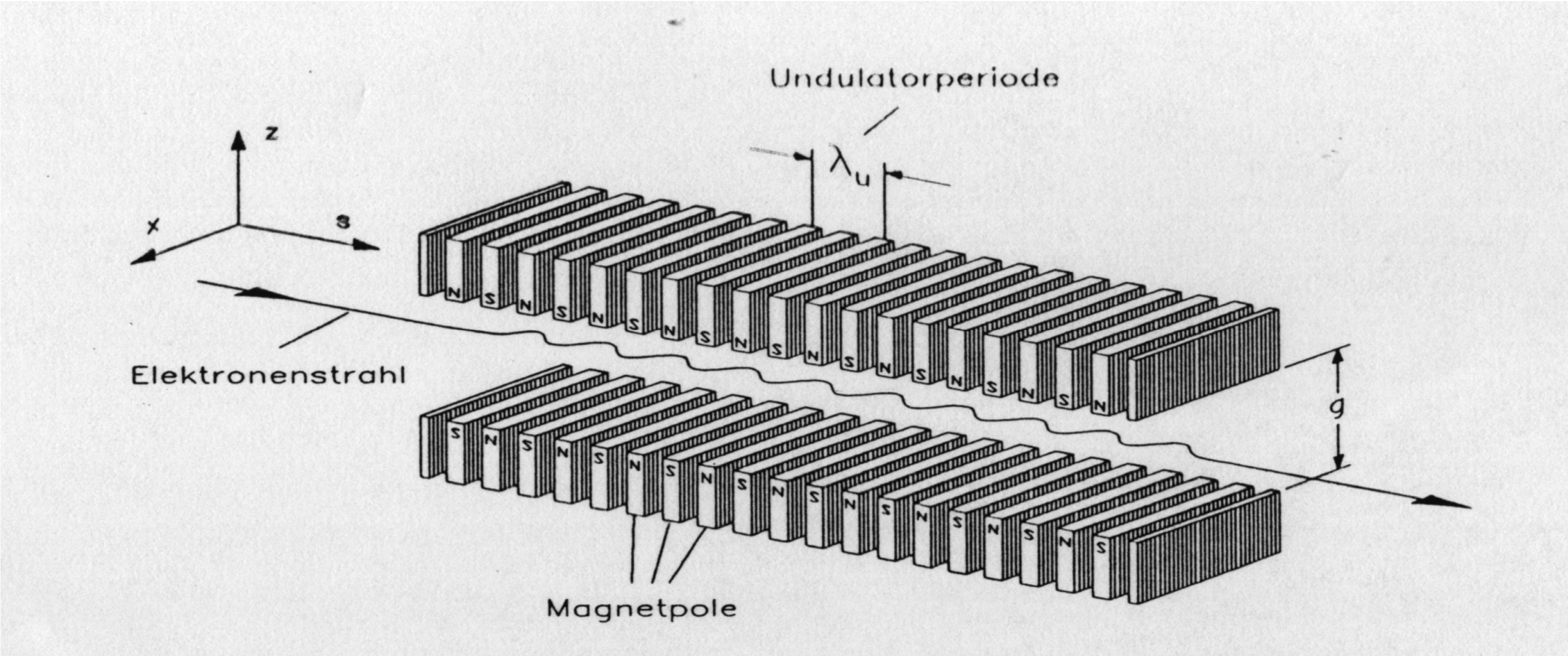
Electron rest frame: **Hertz-Dipole** ⟹ Lab frame: Lorentz-trafo



photon emitted along $\vec{p}_0' = \vec{p}_y'$ ⟹ $\tan\Theta_S = \frac{p_y}{p_z} = \frac{p_0'}{\beta\gamma p_0'} \overset{\beta\approx 1}{\approx} \frac{1}{\gamma}$



How to *shake* (=accelerate) electrons: undulator



$$\vec{F} = m_e \gamma \dot{\vec{v}} = e\vec{v} \times \vec{B}$$ and $$\vec{B} = \begin{pmatrix} 0 \\ B_z \\ B_s \end{pmatrix}; \quad \vec{v} = \begin{pmatrix} v_x \\ 0 \\ v_s \end{pmatrix} \longrightarrow \dot{\vec{v}} = \frac{e}{m_e \gamma} \begin{pmatrix} -v_s B_z \\ -v_x B_s \\ -v_x B_z \end{pmatrix}$$

Lorentz-force

thus, ***coupled*** motion:

$$\ddot{x} = -\dot{s}\frac{e}{m_e \gamma} B_z(s)$$

$$\ddot{s} = \dot{x}\frac{e}{m_e \gamma} B_z(s)$$

K-Parameter

from $\ddot{x} = -\dot{s}\dfrac{e}{m_e\gamma}B_z(s), \quad \ddot{s} = \dot{x}\dfrac{e}{m_e\gamma}B_z(s)$

with $B_z(s) = \tilde{B}\cos(k_u s); \quad \dot{x} = x'\beta c, \quad \ddot{x} = x''\beta^2 c^2$

$$x'(s) = \frac{\lambda_u e\tilde{B}}{2\pi m_e \gamma c}\sin(k_u s) \quad \Rightarrow \quad \Theta_{\max} = x'_{\max} = \frac{1}{\gamma}\frac{\lambda_u e\tilde{B}}{2\pi m_e c}$$

Undulator period → λ_u

Magnetic field strength → $\tilde{B}$

$$K = \frac{\lambda_u e\tilde{B}}{2\pi m_e c}$$

Undulator: $K \leq 1$

Wiggler: $K > 1$

$$\Theta_W = \frac{K}{\gamma}$$

synchrotron radiation:

$$\Theta_S = \frac{1}{\gamma}$$

undulator:

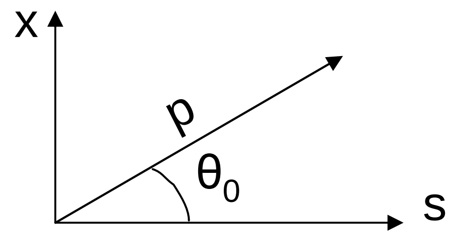
constructive interference due $\Theta_W < \Theta_S$ → **coherence**

(compare with laser amplitude) $a = \dfrac{eE\lambda}{2\pi mc^2} \overset{E=cB}{=} \dfrac{eB\lambda}{2\pi mc}$

Relativistic Doppler Effect:
Transformation from *Co-Moving* System into *Lab* System

$$E = \hbar\omega = pc$$

$$p = \frac{\hbar\omega}{c}$$



Lab system

$$P_{lab} = \begin{pmatrix} E/c \\ p_x \\ p_z \\ p_s \end{pmatrix} = \begin{pmatrix} E/c \\ p\sin\theta_0 \\ 0 \\ p\cos\theta_0 \end{pmatrix}$$

$$P_{co-moving} = \begin{pmatrix} E^*/c \\ p_x^* \\ p_z^* \\ p_s^* \end{pmatrix} = \begin{pmatrix} \gamma^* & 0 & 0 & -\beta^*\gamma^* \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ -\beta^*\gamma^* & 0 & 0 & \gamma^* \end{pmatrix} \begin{pmatrix} E/c \\ p\sin\theta_0 \\ 0 \\ p\cos\theta_0 \end{pmatrix}$$

Lorentz-Trafo

$$\frac{E^*}{c} = \gamma^* \frac{E}{c} - \beta^*\gamma^* p\cos\theta_0 = \gamma^* \frac{\hbar\omega_w}{c}(1-\beta^*\cos\theta_0)$$

$$\text{with } E^* = \hbar\omega^* \Rightarrow \frac{\hbar\omega^*}{c} = \gamma^* \frac{\hbar\omega_w}{c}(1-\beta^*\cos\theta_0) \Rightarrow \omega_w = \frac{\omega^*}{\gamma^*(1-\beta^*\cos\theta_0)}$$

Undulator: fundamental frequency

- transverse oscillation in **lab** system: $\Omega_w = \frac{2\pi}{T} = \frac{2\pi\beta c}{\lambda_u} = k_u \beta c$
- in mean **electron** frame: $\omega^* = \gamma^* \Omega_w$

- undulator radiation observed in **lab** system under angle Θ_0:

relativistic Dopplereffect: $\omega_w = \frac{\omega^*}{\gamma^*(1-\beta^* \cos\Theta_0)}$

with **mean** velocity: $\beta^* = \frac{\dot{s}}{c} = 1 - \frac{1}{2\gamma^2}\left[1 + \frac{K^2}{2}\right]$

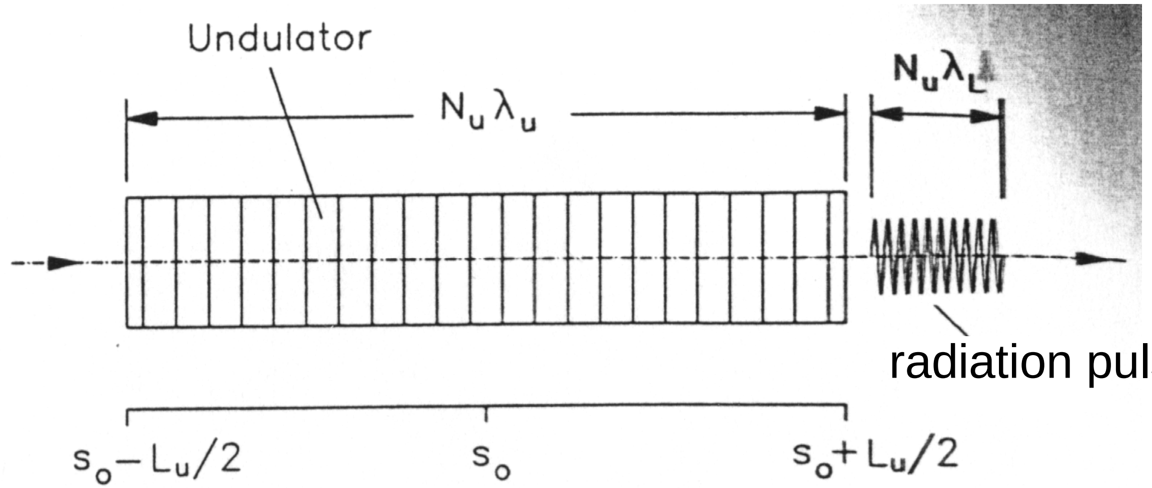
$$\lambda_w = \lambda_u \frac{\Omega_w}{\omega_w} = \lambda_u (1-\beta^* \cos\Theta_0) = \frac{\lambda_u}{2\gamma^2}(1 + \frac{K^2}{2} + \gamma^2\Theta_0^2)$$

- thus,

$$\Rightarrow \boxed{\lambda_w = \frac{\lambda_u}{2\gamma^2}(1 + \frac{K^2}{2} + \gamma^2\Theta_0^2)}$$

(most important equation)

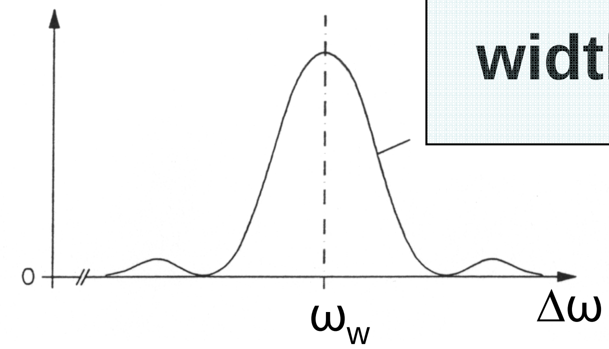
Undulator: Spectral Width



finite duration: $T = N_u \lambda_w / c$ with frequency ω_w

⇨ **continuous** spectrum of partial waves:

$$A(\omega) \sim \frac{\sin(\pi N_u \frac{\Delta\omega}{\omega_w})}{\pi N_u \frac{\Delta\omega}{\omega_w}}$$



width $= \frac{2\Delta\omega}{\omega_w} \approx \frac{1}{N_u}$

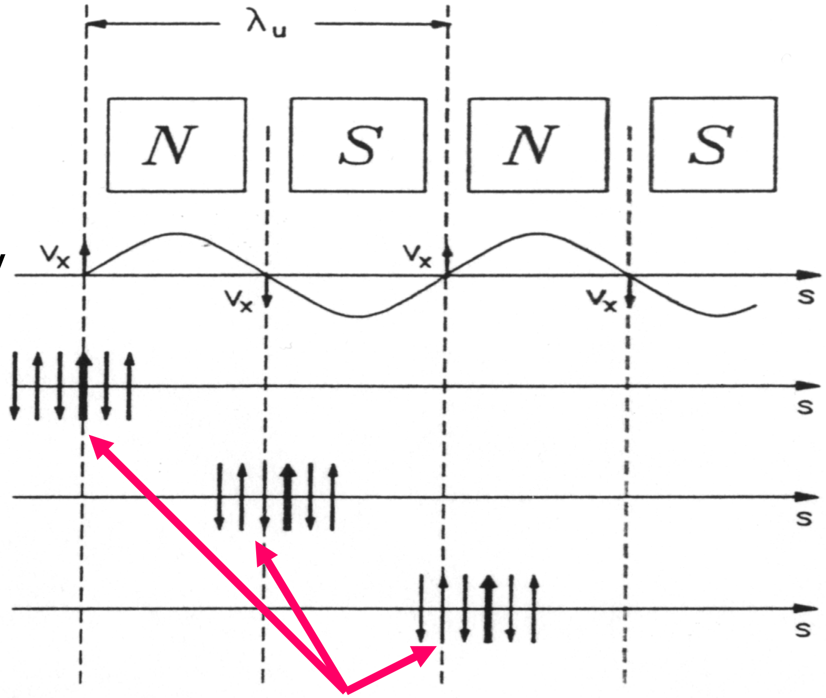
FEL basics: most fundamental point

coherence condition

undulator

electron trajectory

radiation field



electron **transverse motion** in phase with **radiation** phase: $\vec{v} \parallel \vec{E}_L$

this means a net energy transfer from the kinetic energy of the electrons to the radiation field over the total undulator length

FEL basics

electron-laser **interaction**: $\Delta W = -e\int \vec{E}_L d\vec{s} = -e\int \vec{v}\vec{E}_L dt$

electric laser field vector

⟹ coupling via transverse motion: $\vec{v} \parallel \vec{E}_L$

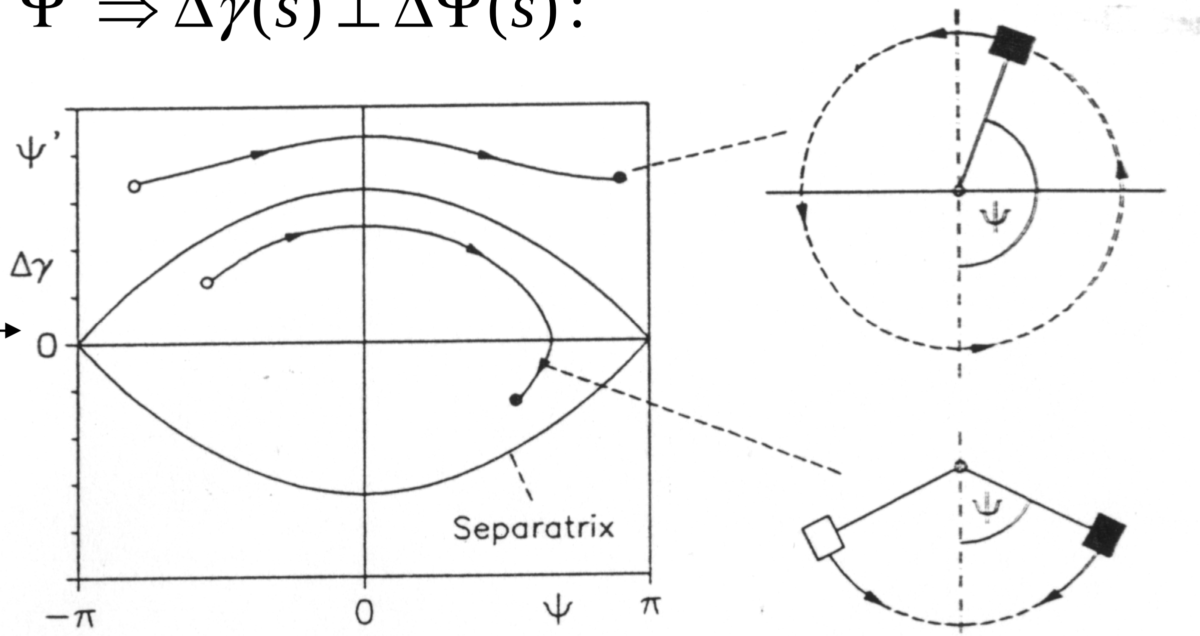
⟹ phase Ψ between electron and radiation **must not** vary

⟹ $\langle \Delta W \rangle \neq 0 \Leftrightarrow \frac{d\Psi}{dt} \approx 0 \Rightarrow \quad \lambda_L = \frac{\lambda_u}{2\gamma^2}\left(1+\frac{K^2}{2}\right)$ ← as known from *undulator* radiation

⟹ $\Delta\gamma \propto \Psi' \Rightarrow \Delta\gamma(s) \perp \Delta\Psi(s):$

Change in electron kinetic energy

usual phase space in FEL theory →



pendulum like motion

Low-Gain/High-Gain

- Gain: $$G = \frac{\gamma_A - \bar{\gamma}}{\gamma_A}$$ ← loss of kinetic electron energy = gain of radiation field

- effect of laser-field, in analogy to K: $$K_L = \frac{eE_{L,0}}{k_u m_e c^2}$$

$$(K_L = a!)$$

$$\boxed{\frac{d\gamma}{ds} \propto \frac{K_L K}{\gamma}}$$

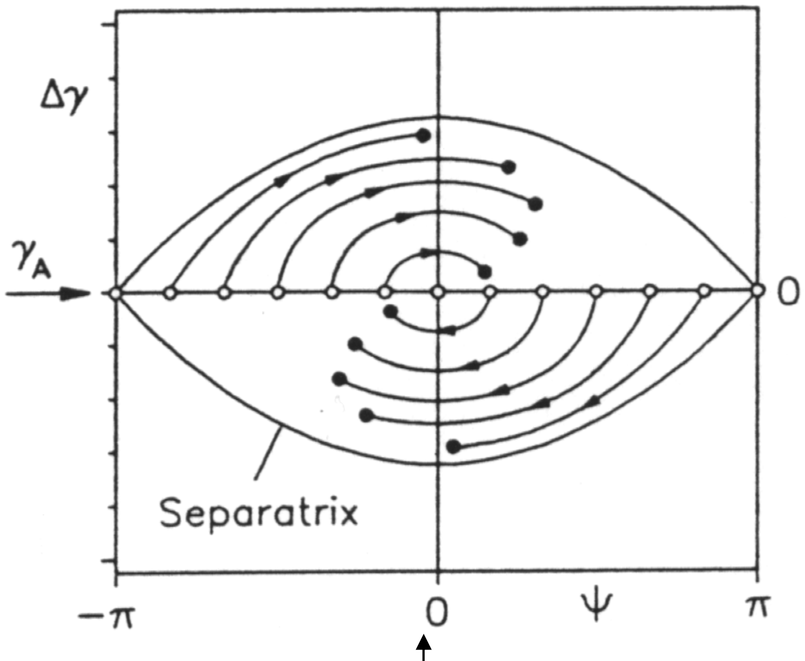
← coupling between electron motion and radiation field

- Low-Gain: K_L small → G few percent

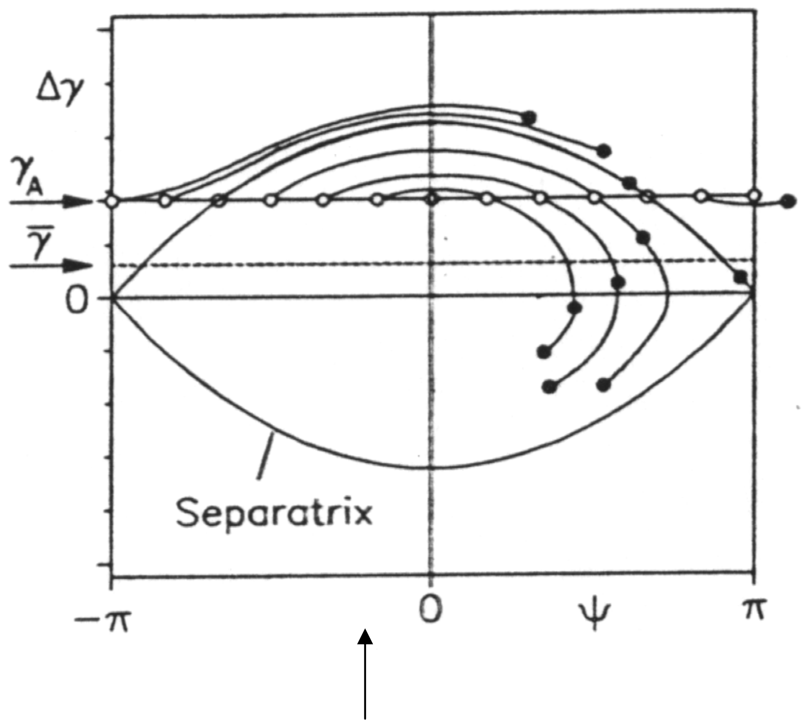
- High-Gain: K_L large → many electrons within separatrix → laser field ≠ const, G large

Initial Energy in Low Gain Regime

operating slightly above resonance energy:



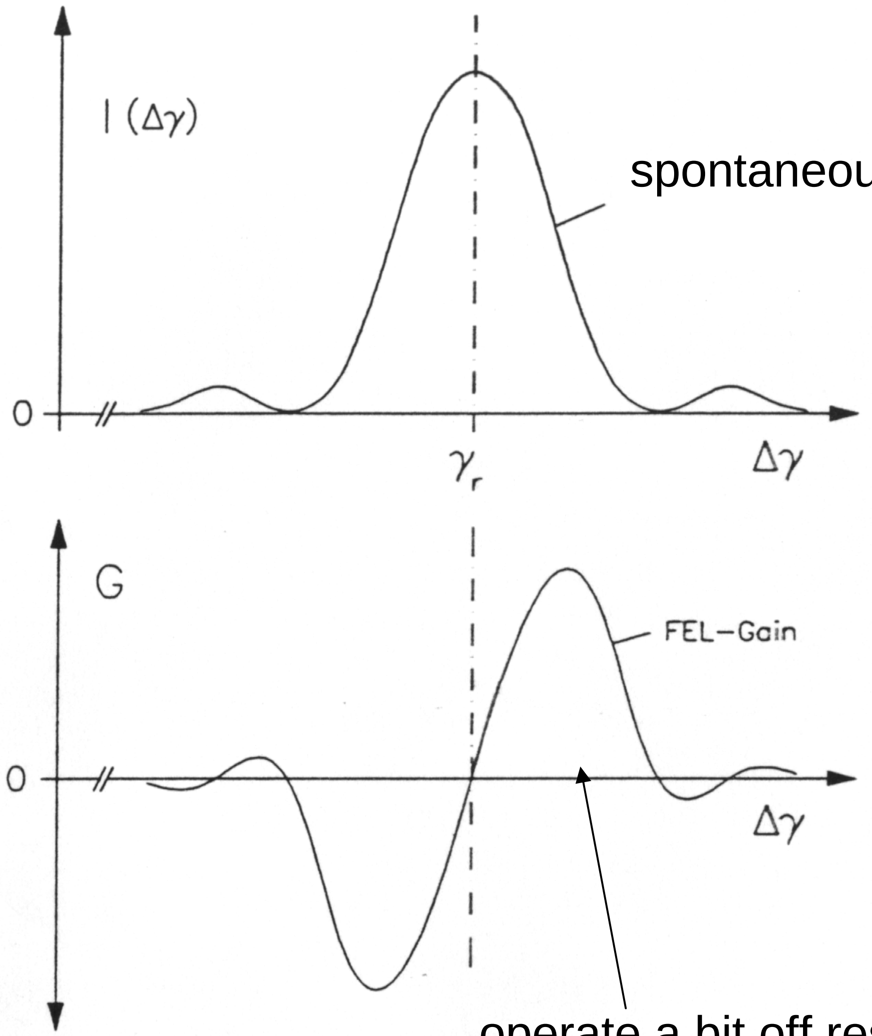
no over-all effect



net effect: electrons transferred energy to radiation field

Madey Theorem

Madey-theorem: Gain is derivative of spontaneous spectrum

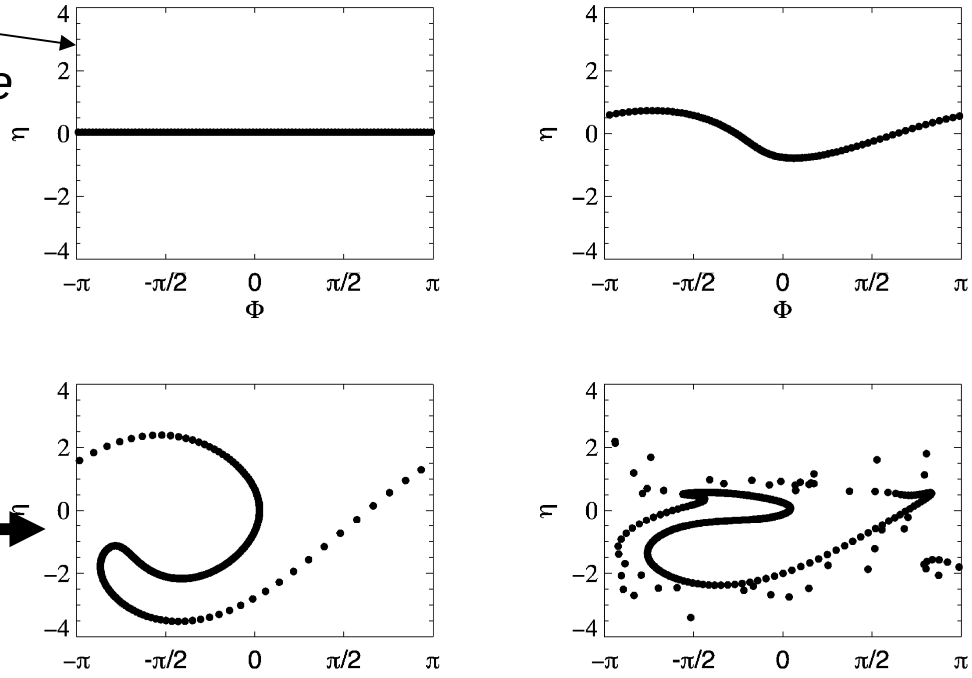


valid only for
low-gain regime

operate a bit off resonance, where max gain!

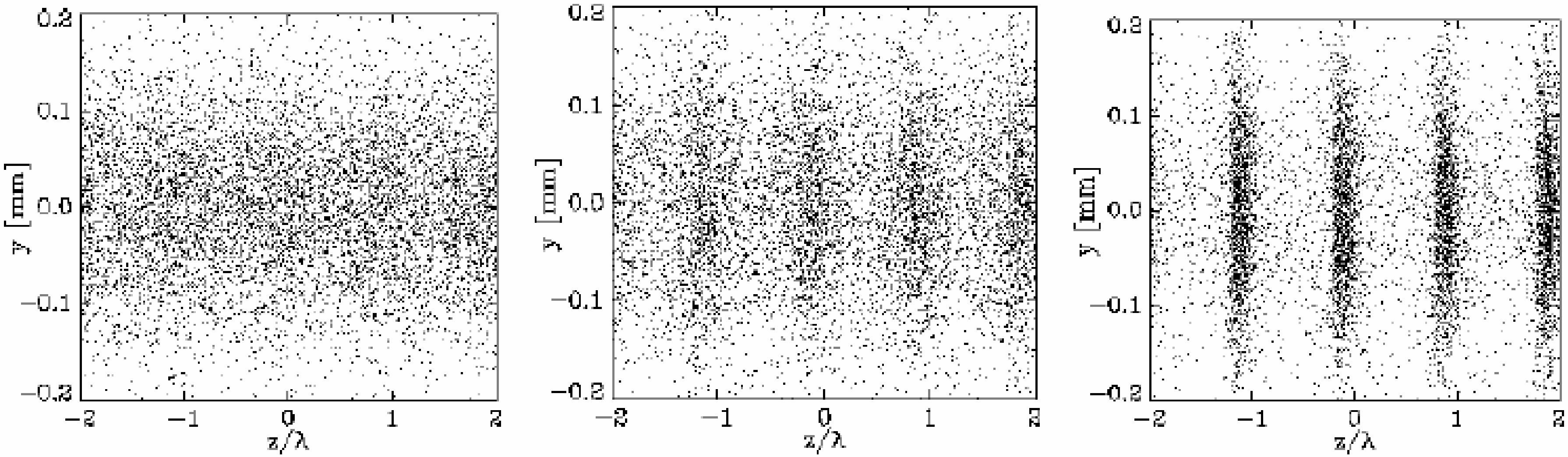
High Gain: SASE-FEL and micro-bunching

Same phase space as before



- **SASE=S**elf-**A**mplification of **S**pontaneous **E**mission
- **no seeding** field
- strong **micro-bunching**

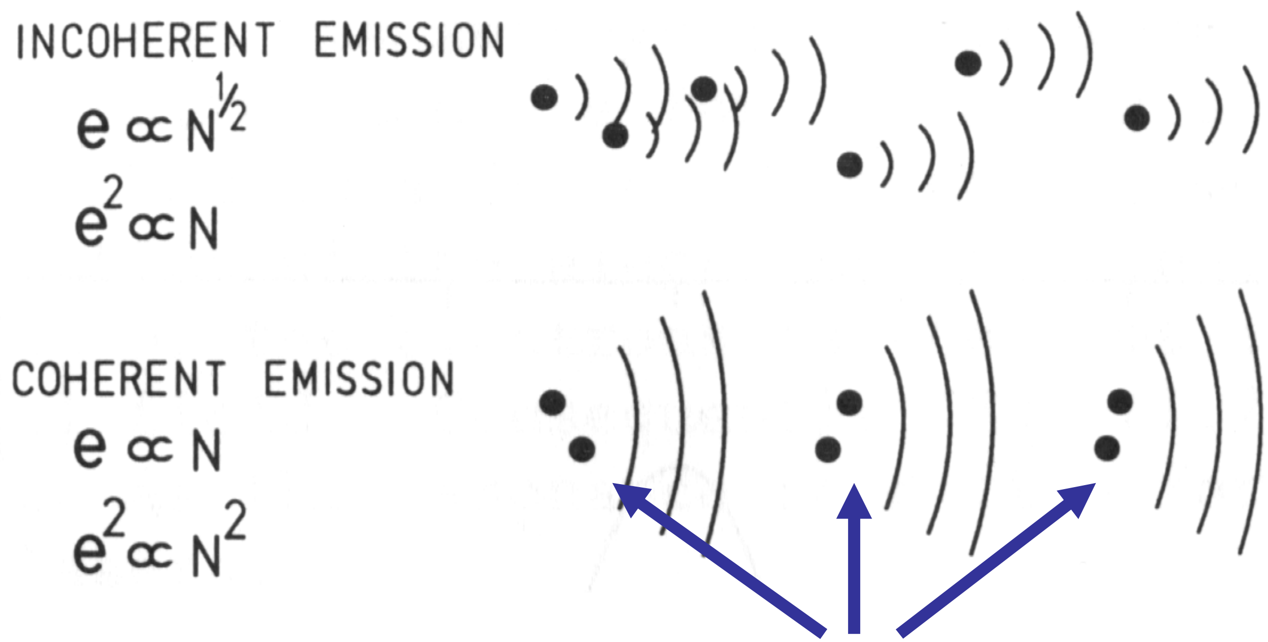
  = 90° rotation in phase-space



SASE-FEL: *coherent radiation*

incoherent emission amplitude *e* from **random walk**

(intensity ~ amplitude²)



Micro-bunching! → coherent emission

note: N ~ 10^{10} !!!!

The FEL Instability

Induced **energy** modulation

Increasing **density** modulation

Run-away process
(**collective instability**)

Enhanced **emission**

The FEL process **saturates** when maximum density modulation (bunching) is achieved.

Characteristic Parameter: Pierce

- everything scales with the so-called **Pierce** paramter
- in FEL theory there is a 1d- and 3d-Pierce parameter

- **ideal** 1d-Pierce parameter:

$$\rho = \left[\left(\frac{I}{I_A} \right) \cdot \left(\frac{\lambda_u A_u}{2\pi\sigma_x} \right)^2 \left(\frac{1}{2\gamma} \right)^3 \right]^{1/3}$$

electron current (I); *Alven current = 17 kA* (I_A); *undulator period* (λ_u); *~ K (undulator parameter)* (A_u); *electron beam diameter* (σ_x)

- typically $\rho \sim 10^{-4 \ldots -3}$
- **real** beams have energy spread and emittance….

Realistic gain length

- **ideal** gain length : $L_{1d} = \lambda_u / (4\pi\sqrt{3}\rho)$

- from FEL analysis: $$\frac{L_{1d}}{L_g} = F(\eta_d, \eta_\varepsilon, \eta_\gamma)$$

diffraction $$\eta_d = \frac{L_{1d}}{L_r}, \text{ with } L_r = 4\pi\sigma_x^2 / \lambda$$

emittance $$\eta_\varepsilon = \left(\frac{L_{1d}}{\beta}\right)\left(\frac{4\pi\varepsilon}{\lambda}\right)$$

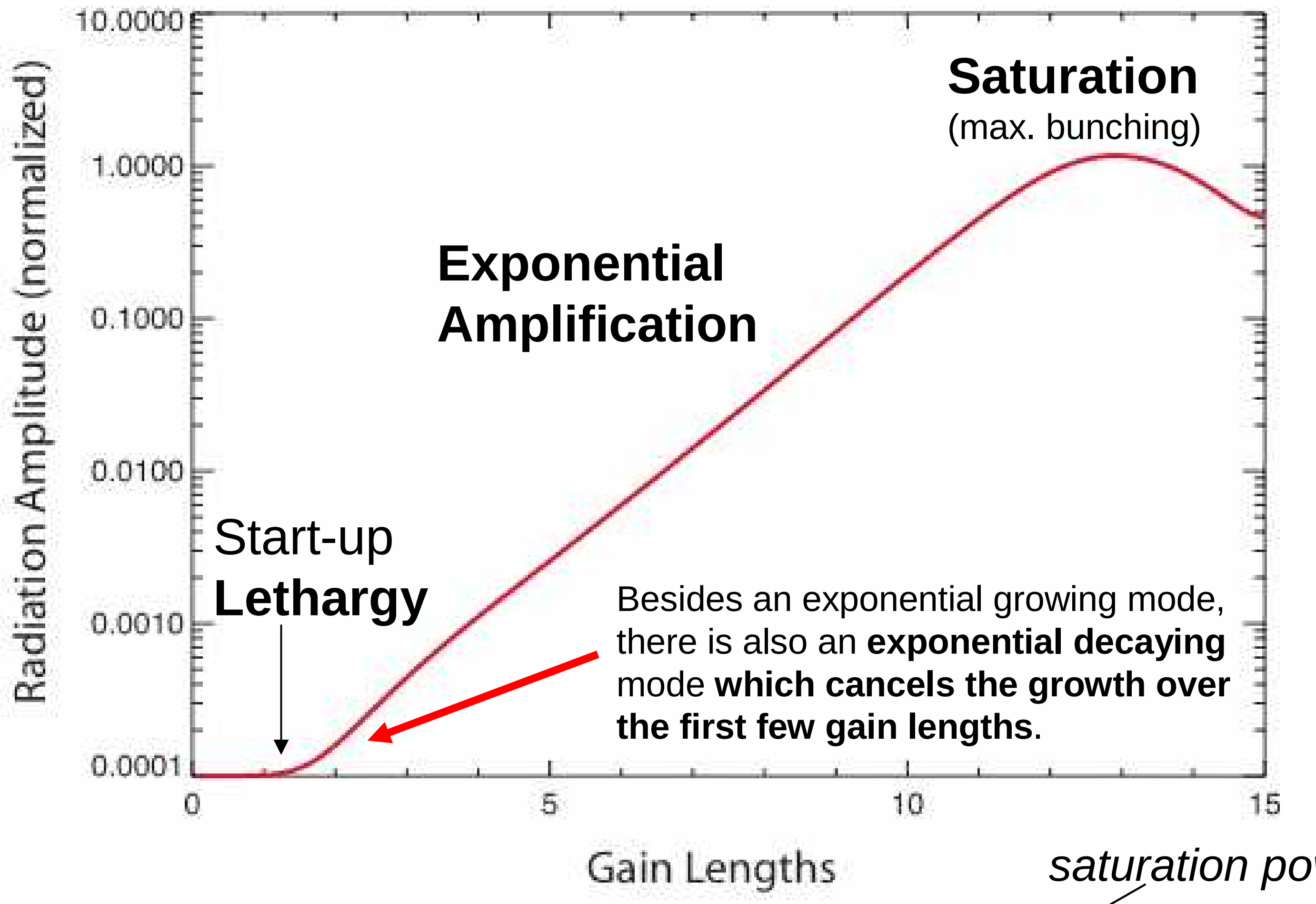
emittance [mm.mrad]

focusing: $\sigma_x^2 = \beta\varepsilon$

energy spread $$\eta_\gamma = 4\pi\left(\frac{L_{1d}}{\lambda_u}\right)\left(\frac{\sigma_E}{E_0}\right)$$

energy spread

Saturation length



undulator length should be saturation length:

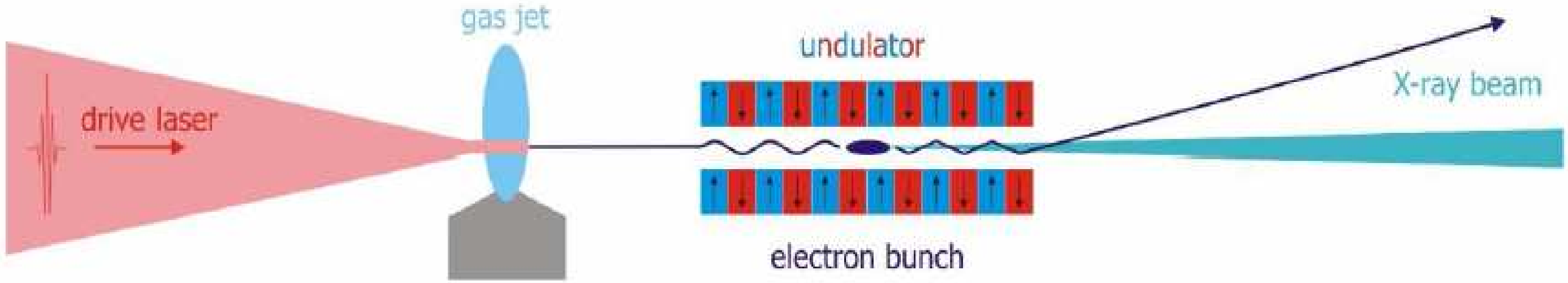
saturation power

$$L_{sat} = L_g \cdot \ln\left(\frac{P_{sat}}{\alpha \cdot P_{noise}}\right) \approx 15 \cdot L_g$$

spontaneous power after one gain length

...in practice: *table-top FELs*

experimental setup:



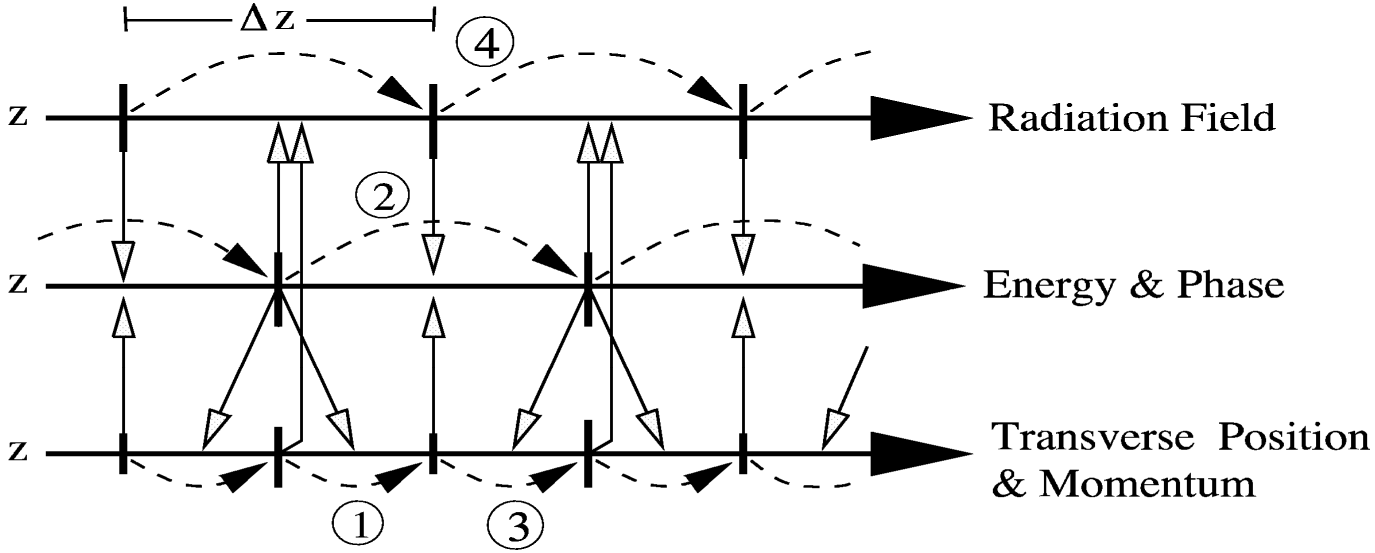
How to **design** something like that?

- FEL simulation (see next): same as for DESY+SLAC
- undulator design ("EM-studio")
- electron tracking ("waves" + "GPT")
- bubble: PIC code ("VPL" + "ILLUMINATION")
- in future: "S2E" = start-to-end simulation

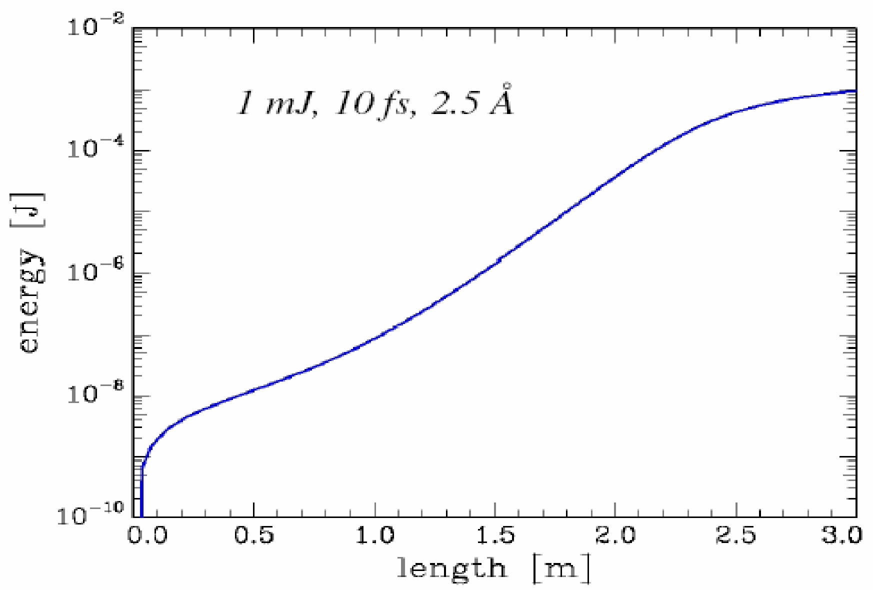
"GENESIS 1.3" code

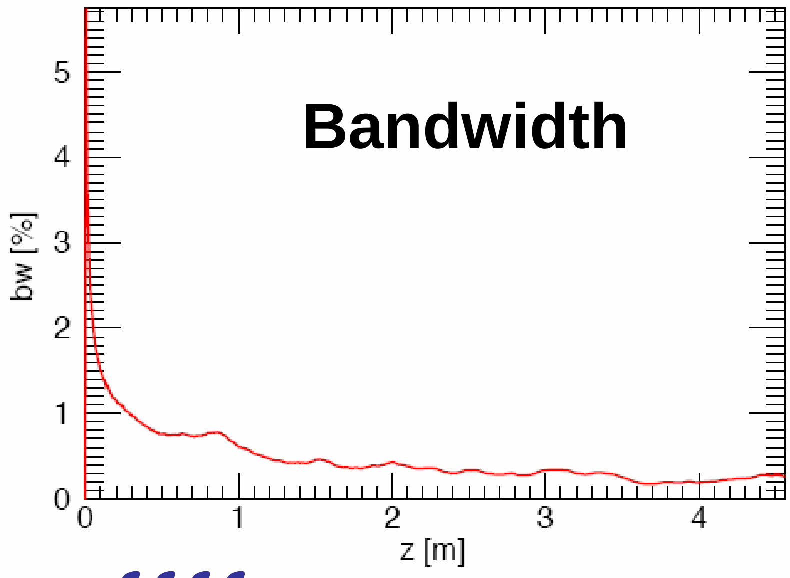
code for SASE-FEL simulation:

- author: Sven Reiche (DESY, UCLA)
- based on **FEL** equations
- **not** a PIC code
- covers cm and nm scales
- explicit integration over undulator period: $\Delta z = \lambda_U$

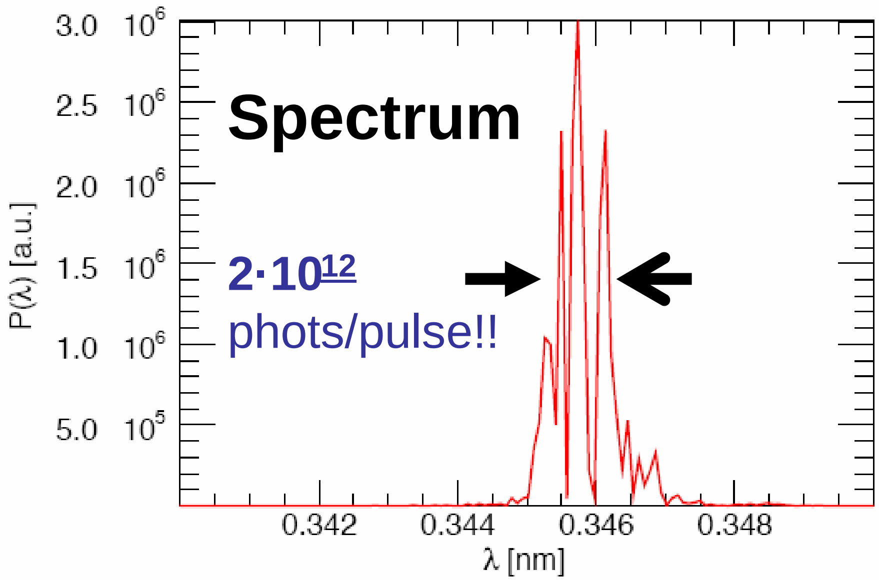


Full simulation of "TT-XFEL"



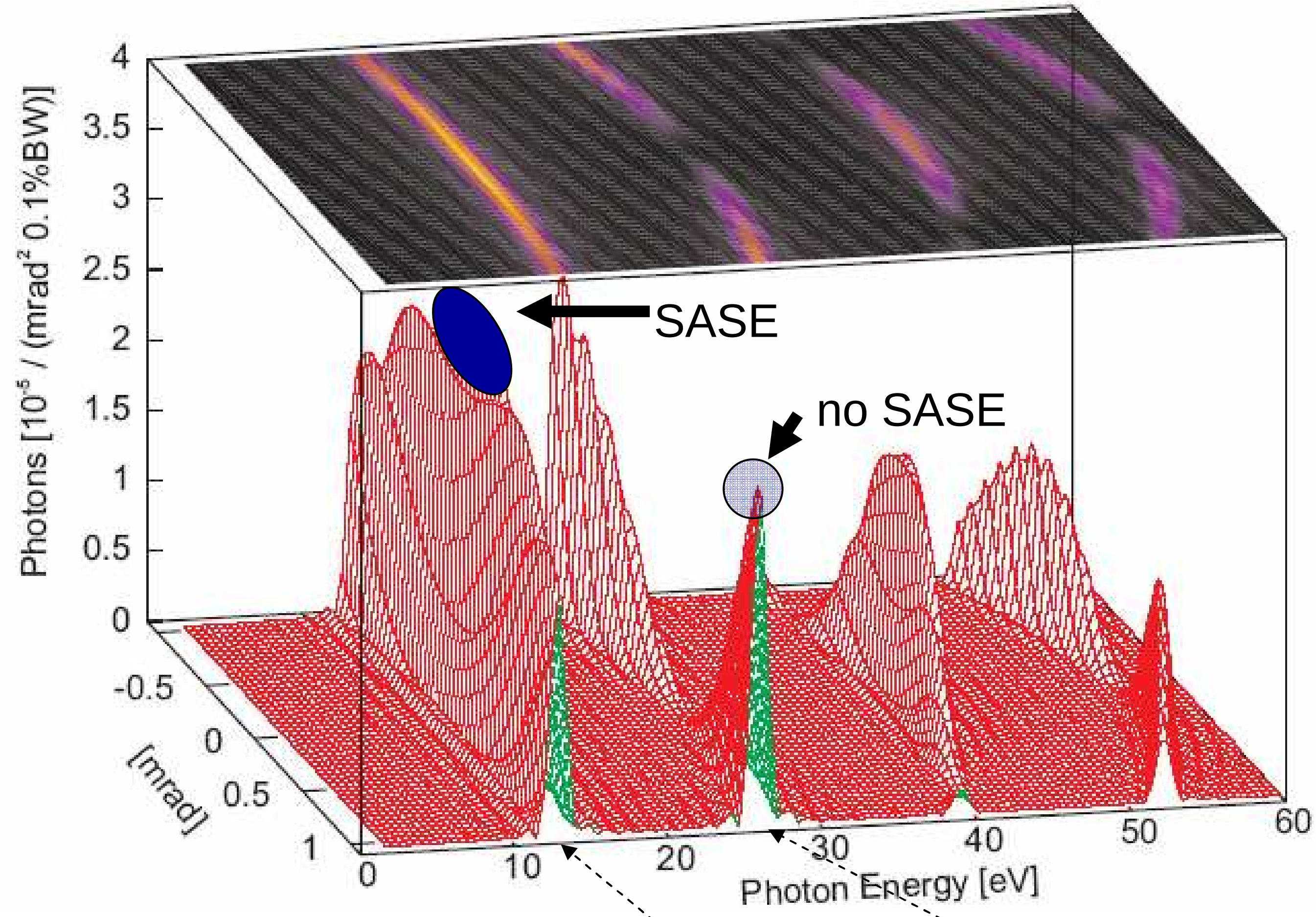


It's lasing !!!!



charme of our concept:
3 meter only!!!!

…but, before, just *proof-of-principle*…



take measured **reference spectrum** (unfolded for energy spread and emittance) and compare **ratios of fundamental to first harmonic**

on-axis **off-axis**