

Post-saturation Dynamics and Superluminal Propagation of a Super-radiant Spike in a Free-Electrons Laser Amplifier

Xi Yang¹, Najmeh Mirian² and Luca Giannessi^{2,3}

¹National Synchrotron Light Source II, Brookhaven National Laboratory, Upton, New York 11973, USA

²Elettra-Sincrotrone Trieste, Strada Statale 14-km 163,5, 34149 Basovizza, Trieste, Italy and

³ENEA Frascati, Via Enrico Fermi 45, 00044 Frascati, Italy

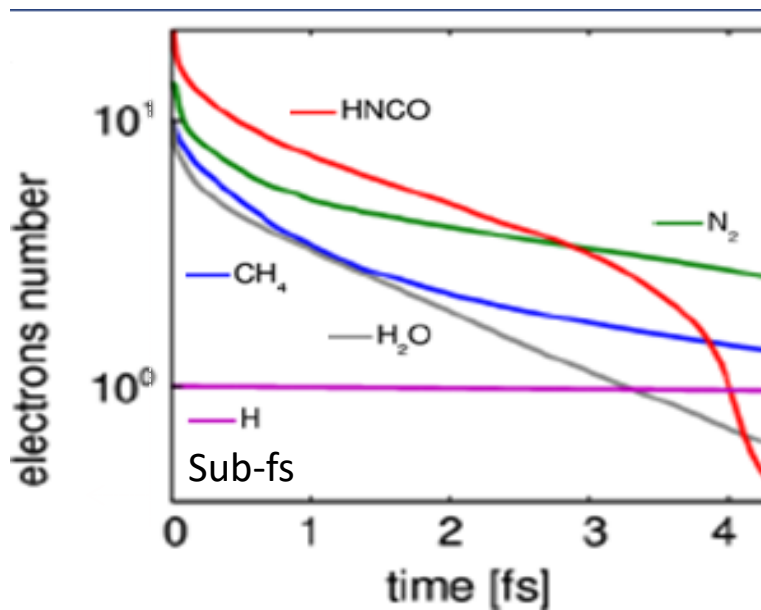
Outline

- Brief overview of methods to achieve ultrashort pulses or single spike in FELs at saturation
- Investigation of pulse structure using a numerical approach based on PERSEO (no analytical solution available)
- Saturation effects
 - Pulse shortening and power increasing
 - Pulse splitting and tail formation
 - Main peak moving at *superluminal* velocity ($v_g > c$)
- The pulse has a tail .. tail structure
 - FEL pulse splits into the front (ζ_+) and trailing (ζ_-) modes after saturation
- Tail suppression
 - Optimize energy spread ($\sim \frac{\rho_{fel}}{2}$) and energy spread tapering via a laser heater

Motivation for Single-Shot Isolated-Molecule Imaging

- Key issues:
 - Time scale (sub-fs): Acquiring single-shot images before radiation damage/Coulomb explosion of the sample takes place
 - Spatial resolution: Resolving the structure of proteins that cannot be crystallized in single-molecule level
 - High Intensity: 10^{11} photon/pulse at $P=150$ GW, $\lambda=0.4$ nm with $\sigma_{t\text{-FWHM}}=400$ as
- Such conditions can be met by XFEL with peak power of multi-GW and sub-fs temporal duration

Number of “bounded” electrons versus time of molecules illuminated by XFEL radiation with power $P=150$ GW and $\lambda = 0.4$ nm



A. Fratalocchi and G. Ruocco
PRL 106, 105504 (2011)

Methods to Achieve Single Spike @ Saturation

- There are a number of ways to trigger the formation of an ultrashort single spike in a FEL amplifier:
 - Short electron bunch single spike J. Rosenzweig *et al*, NIMA 593(2008)
 - Chirp + Taper
200 as (FWHM) and 100 GW in $\lambda \sim 1\text{\AA}$ (sim) E. Saldin *et al*, PRST-AB 9, 050702 (2006)
 E_{out} increases >10 times in single spike SASE at $\lambda \sim 540\text{nm}$ (exp) L. Giannessi *et al*, PRL 106, 144801 (2011)
 - Slotted foil
Sub-fs 10GW x-ray pulse P. Emma *et al*. PRL 92, 074801 (2004)
 - Multi-foil + Electron Delay
500as (FWHM) and 1TW at $\lambda \sim 1\text{\AA}$ (sim) E. Prat and S Reiche PRL 114, 244801 (2015)
 - Fresh bunch self-seeding
50 GW, 9 fs at 5.5keV C. Emma *et al*, APL 110, 154101 (2017)
 - Chirp + Taper + Fresh bunch self-seeding
0.5TW and 260as (FWHM) at $\lambda = 1.5\text{nm}$ S. Huang *et al*, PRAB 19, 080702 (2016)

We investigated the dynamics of this spike when it reaches saturation in a simplified model – uniform current – no energy spread (in the beginning)

Saturation of the single spike

- Saturation is reached when the peak power exceeds $\sim 1.6\rho P_e$
- Flat current model -> The pulse propagates over «fresh electrons»
- Superradiance*
 - Modifying the pulse properties due to the electron longitudinal synchrotron oscillations.
 - Scaling relations**: $P_L \propto z^2, E_L \propto z^{3/2}, \sigma_t \propto z^{-1/2}$

*R. Bonifacio, B. W. J. Mc Neil, P. Pierini, PRA 40, 4467 (1989)

R. Bonifacio, L. De Salvo Souza, P. Pierini, N. Piovella, NIM A296, 358 (1990)

** see: L. Giannessi, P. Musumeci, S. Spampinati, JAP 98, 043110 (2005)

Experiments: Watanabe et al. PRL 98, 034802 (2007)

SPARC, Frascati: PRL 106, 144801 (2011) – PRL 108, 164801 (2012) – PRL 110, 044801 (2013)

Coupled Maxwell-Lorentz equations in the slowly varying envelope approximation

$$\frac{\partial \theta_j}{\partial u} = v_j, \frac{\partial v_i}{\partial u} = -[a(\zeta, u) \cdot e^{i\theta_j} + c.c.],$$
$$\left(\frac{\partial}{\partial u} + \frac{\partial}{\partial \zeta}\right) a(\zeta, u) = -b(\zeta, u).$$

Equation (1)

$$\theta_j = [(k_u + k_r)(l_2\zeta + l_1u) - k_rl_1u/\beta_z], \quad u = \beta_z ct/l_1, \zeta = (z - \beta_z ct)/l_2, \quad l_{1,2} = \lambda_{u,0}/(4\pi\rho_{fel})$$

Integrate equations (1) using a numerical approach based on the code PERSEO
Our approach is capable of describing the main pulse and trailing pulses in detail

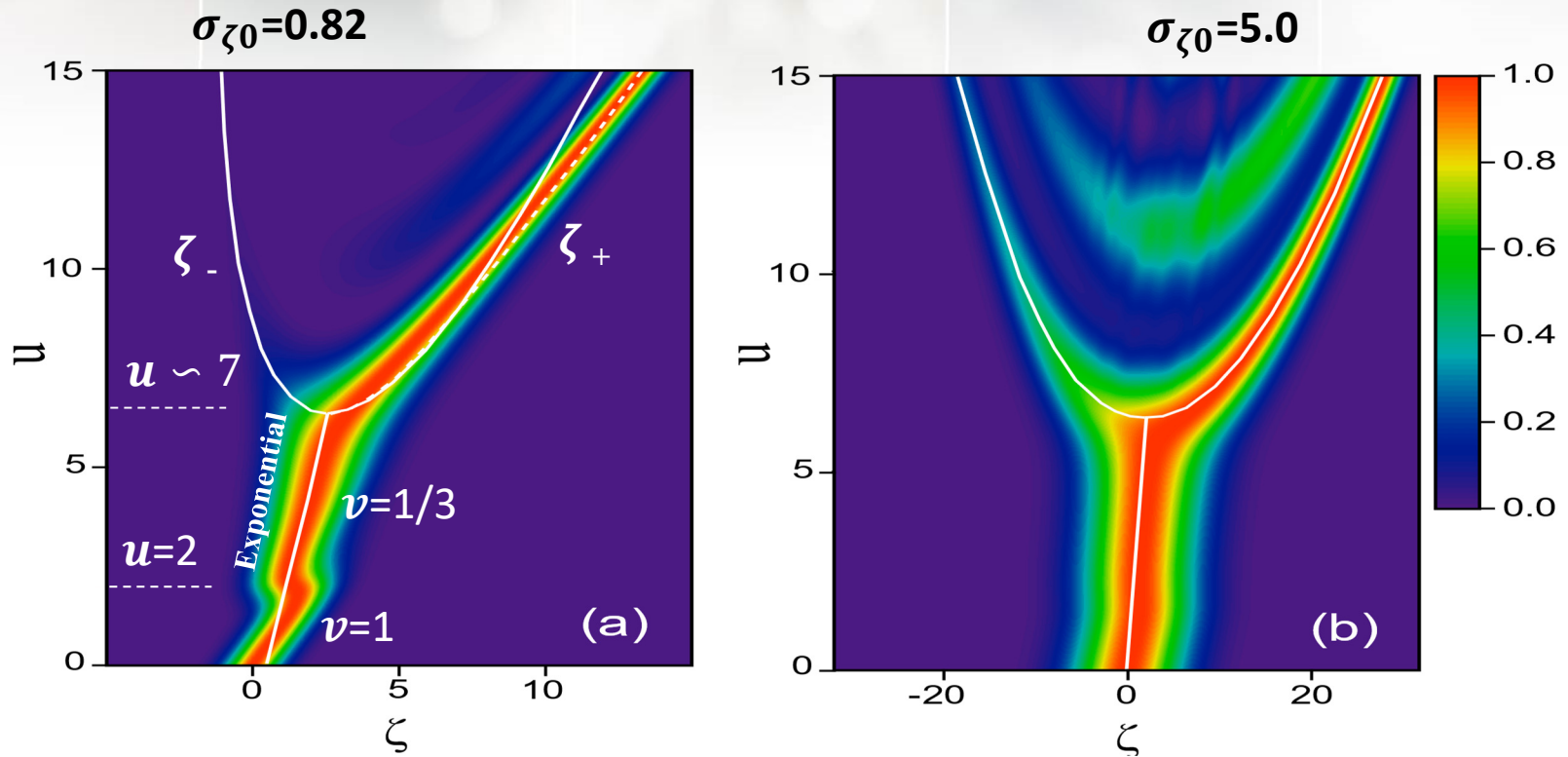
Trigger the formation of an isolated spike by setting the initial condition

$$a(\zeta, 0) = a_0 \cdot \exp\left[-(\zeta - \zeta_0)^2 / 4\sigma_{\zeta_0}^2\right],$$

and imposing “quiet start” to the particle distribution.

$$b(\zeta, 0) = 0. \frac{\partial b(\zeta, 0)}{\partial u} = 0$$

Radiation Power vs ζ, u



- u : Normalized beam position along the undulator.
- ζ : Relative particle position in a frame drifting with the average longitudinal velocity of the e- bunch
- The pulse propagation velocity is given by the slope $\frac{d\zeta}{du}$
- $\sigma_{\zeta 0}$ corresponds to the ratio of gain bandwidth and pulse bandwidth.
- Rear modes strongly depend on this ratio:
 - $\sigma_{\zeta 0} < 1$, rear modes suppressed
 - $\sigma_{\zeta 0} > 1$, rear modes enhanced

Coupled Maxwell-Lorentz equations in the slowly varying envelope approximation

We approximate the field at saturation with a Gaussian drifting with velocity v and growing as

$$|a(\zeta, u)| = a_s \cdot \exp \left[-\frac{(\zeta - v(u - u_s) - \zeta_s)^2}{4\sigma_{\zeta_s}^2} + \frac{\sqrt{3}}{2}(u - u_s) \right]$$

We impose a «local» saturation condition $|a(\zeta, u)| = a_s$

And we find the roots corresponding to the position of the front and rear peaks of the pulse

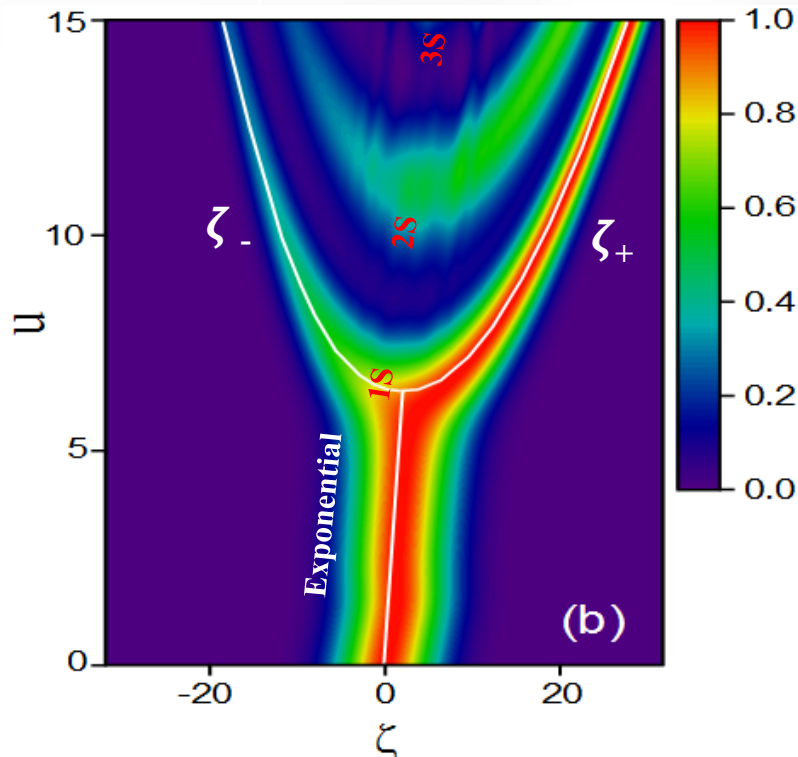
$$\zeta_{\pm}(u) = \zeta_s + (u - u_s)v \pm \sigma_{\zeta_s} [2\sqrt{3}(u - u_s)]^{1/2}$$

Front and rear modes: position $\zeta_{\pm}$ as a function of u

The long seed case ($\sigma_{\zeta 0} > 1$) with two symmetric roots

Pulse splitting in short wavelength seeded FEL

M. Labat *et al* PRL 103, 264801 (2009)



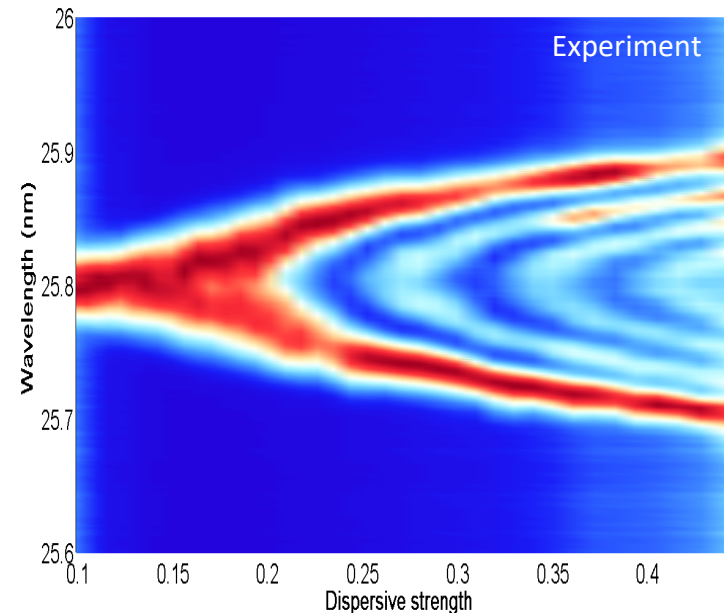
Length of the tail is given by

$$\Delta \sim \zeta_+ - \zeta_- = 2\sigma_{\zeta s} [2\sqrt{3}(u - u_{sat})]^{1/2}$$

The calculated positions of the front and rear peaks match well with simulated peaks

From the FERMI Modulator
with strong chirped seed, spectral map

G. DeNinno et al PRL 110, 064801, 2013
B. Mahieu et al. Optics Express 21, 22728
D. Gauthier et al. Phys. Rev. Lett. 115
D. Gauthier et al. Phys. Rev. A 88



Radiation Power vs ζ, u

- 1) In deep saturation the peak velocity converges to 1 and not to 1/3
- 2) The splitting process still pushes the front peak forward

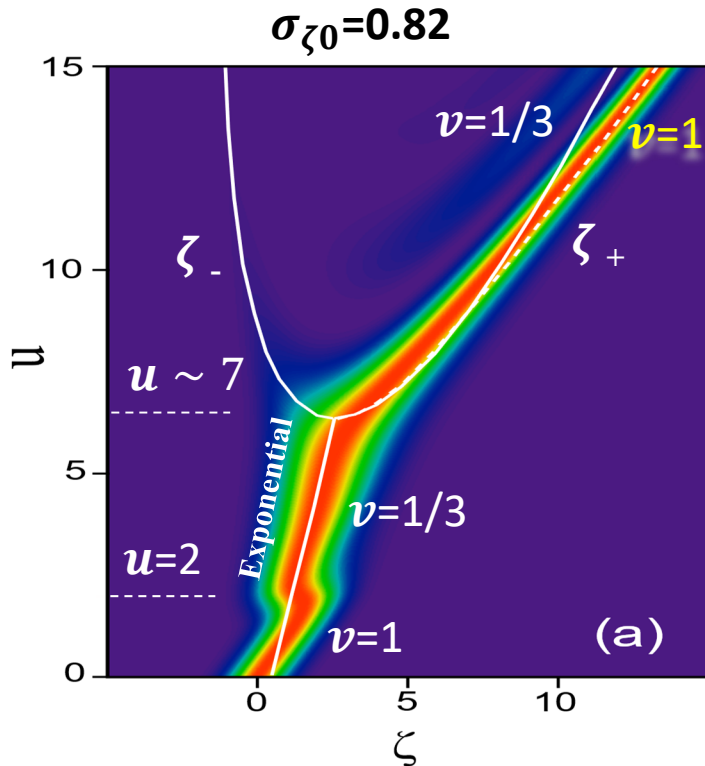
We combine quadratically these two terms modifying

$$\zeta_+(u) - \zeta_s = (u - u_s)v + \sigma_{\zeta_s} [2\sqrt{3}(u - u_s)]^{1/2}$$

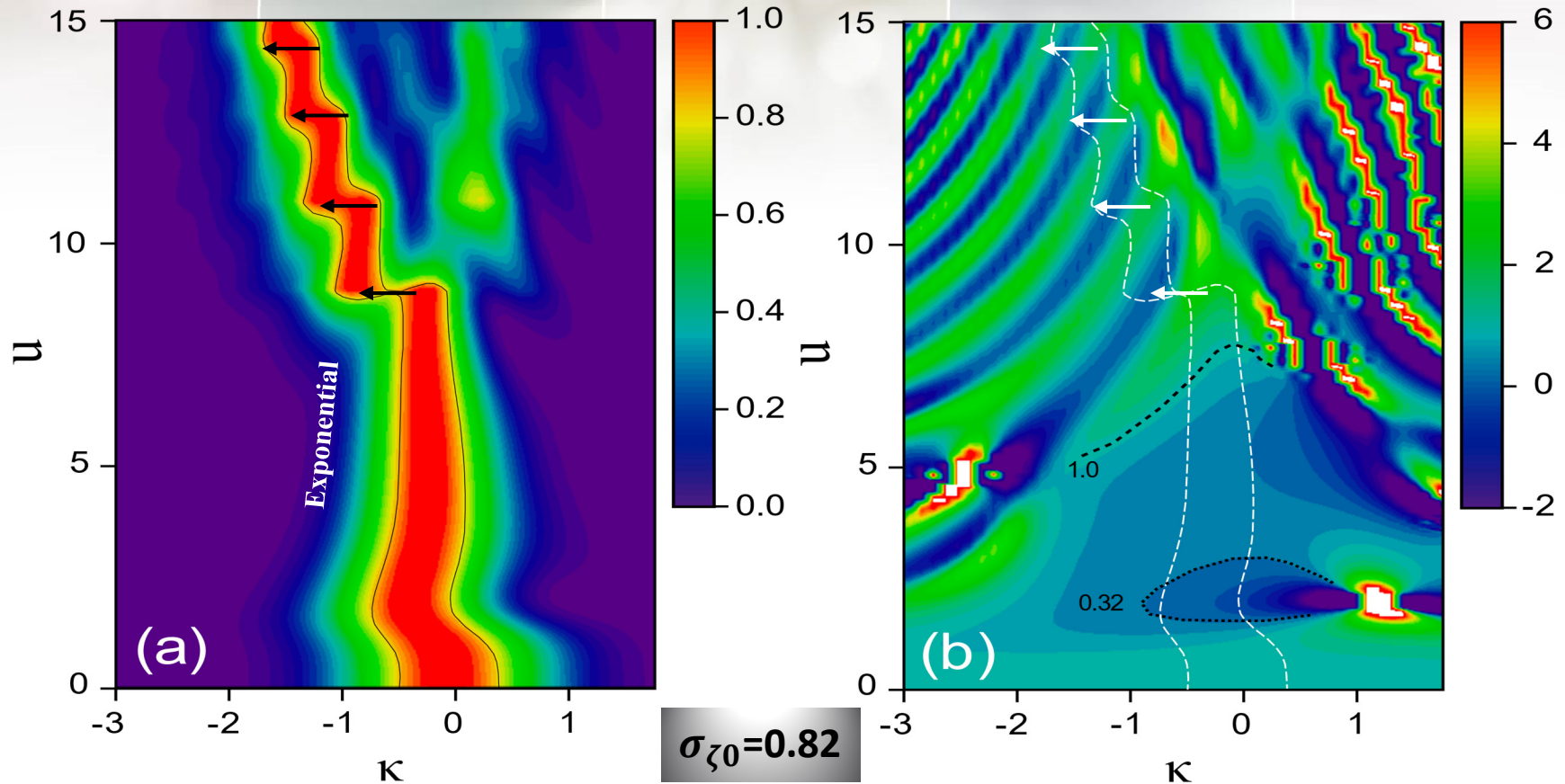
... into

$$\stackrel{v=1}{\Leftrightarrow} \left\{ (u - u_s)^2 + \left[\sigma_{\zeta_s}^2 [2\sqrt{3}(u - u_s)] \right] \right\}^{1/2}$$

... but we have $\frac{d\zeta}{du} > 1$

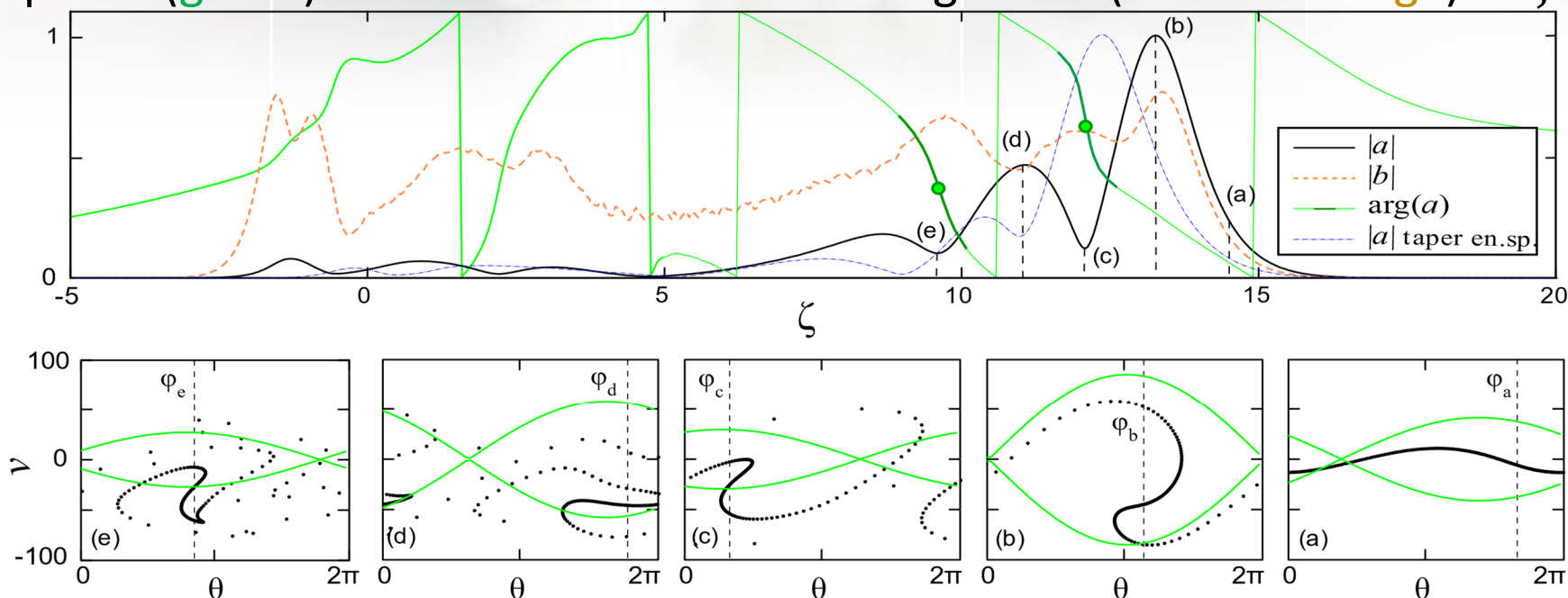


Power Spectrum (left) and Group Velocity (right)



- Group velocity $v_g = \frac{d\omega}{d\kappa} = \frac{d}{d\kappa} \left[\frac{d}{du} \arg(\tilde{a}) \right]$.
 $\tilde{a}(\kappa, u) = \int_{-\infty}^{\infty} \exp(ik\zeta) a(\zeta, u) d\zeta$ is the Fourier transform of the field $a(\zeta, u)$.
 κ is normalized wave-vector $\kappa = (k - k_0)/2\rho_{fel}k_0$.
- Exponential gain process filters the spectrum which narrows up to $u=8$
- $v_g > 1$ at the splitting position ($u=8$), corresponding to red shifted structure
- Radiation energy flows from spectral regions where $v_g > 1$ to where $v_g < 1$ (white dashed line in right plot), corresponding to the discrete red-shifts in the evolution of the spectrum (black solid line in left plot)

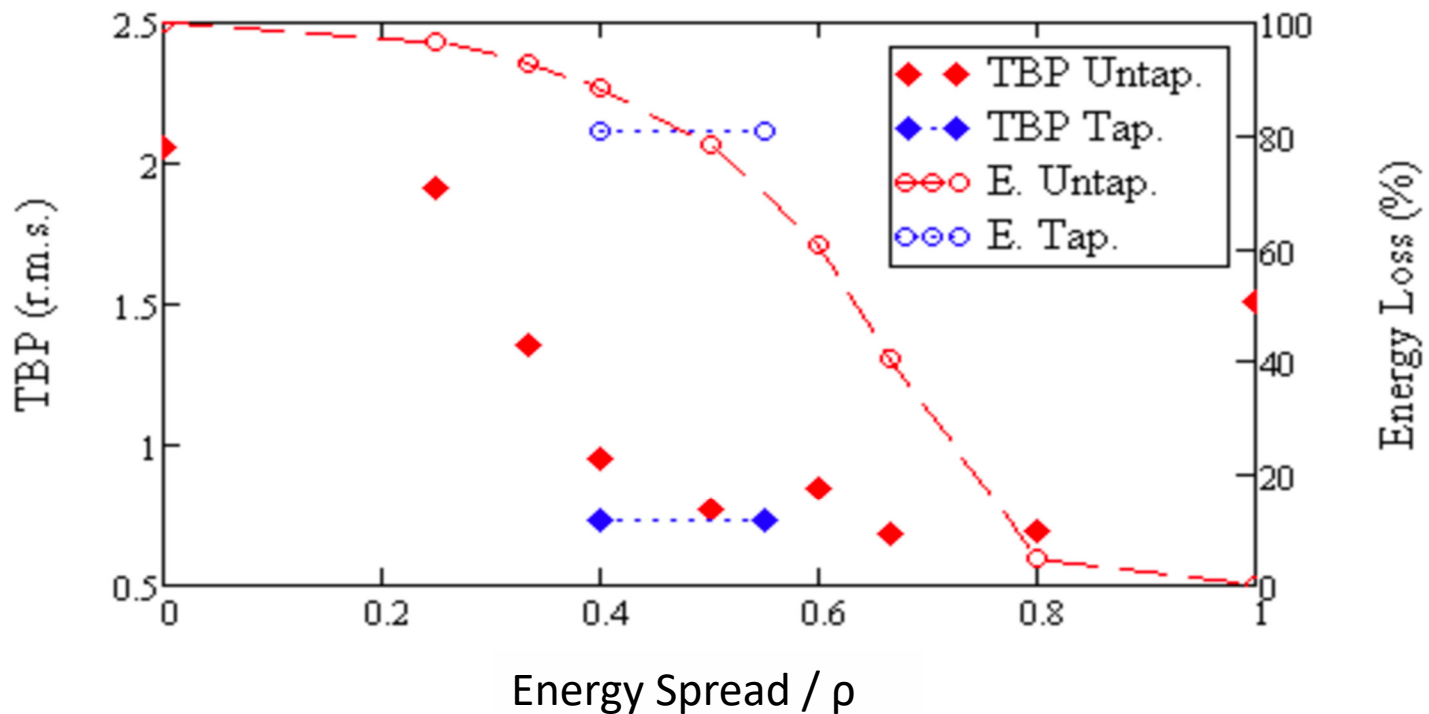
Field amplitude normalized to the main peak with uncorrelated $\sigma_E = 0$ (black)
 optimized case $\sigma_E = \frac{\rho_{fel}}{2}$ with minor energy spread tapering (blue),
 phase (green) and modulus of the bunching factor (dashed-orange) vs ζ



$$S_{\pm} = \pm \sqrt{2 [Re(a) \sin(\theta) + Im(a) \cos(\theta) + |a|]}$$

- Total six peaks. The first 3 on the right side: front side modes, and the 3 in the tail: trailing modes.
- Bunching factor (orange dashed line) is high in the entire pulse region ~ 0.5 .
- The amplitude asymmetry between the two sets of modes: favoring the front side slipping on fresh electrons and radiation power growing as u^2 .
- The phase (light green line) shows a quadratic behavior.
- On the leading edge, peaks (b) and (d), the phase has a linear trend with a phase shift of $\sim \pi$ occurring at the transitions between the sub-pulses, positions (c) and (e) indicated by the dark green.

Time bandwidth product (TBP) (primary-Y) and main pulse energy loss (secondary-Y) as a function of $(\sigma_E/E)/\rho$



- Trailing pulses are influenced by the inhomogeneous broadening associated to beam energy spread σ_E/E .
- An induced beam energy spread reduces energy loss in the tail ($\omega_\Delta = \frac{E_{tail}}{E_{tot}}$) and TBP close to the *Fourier transform limited case* (~ 0.5), but causes a reduction of the pulse energy in the main peak.
- $\sigma_E \cong \frac{\rho}{2}$ reduced $\frac{E_{tail}}{E_{tot}}$ from 23% to 2.5% and TBP from 2.1 to 0.7 with minor energy loss of main peak (20%)
- Tapering σ_E/E with a laser heater or triggering the pulse growth at a specific position along the beam where a larger σ_E/E (adjusting the delay), a minor improvement (blue case).

Summary

- Time-resolved single-shot imaging of isolated molecules or non-periodic structures requires an XFEL with peak power at multi-GW level and sub-femtosecond temporal duration **⇒ FEL operating in single spike - superradiant regime**
- When single spike reaches saturation, pulse splits and tail is formed. We studied this process in ideal conditions, “flat” beam condition
- Peak of **the pulse propagates at superluminal speed at saturation**
The tail is constituted by a train of pulses with both transverse and longitudinal coherence and decaying amplitudes
- **Suppressing the tail to 2% of the main pulse**, can be achieved by inducing additional energy spread $\sigma_E \cong \frac{\rho_{fel}}{2}$. Observed a factor of 3 reduction in TBP and a factor of 10 reduction in E_{tail}/E_{tot}
- Understanding this kind of phenomenon is important to extend the FEL performance to some of the most challenging applications (e.g. resolving the structure of proteins that cannot be crystalized)

«Single electron» FEL amplifier