Molecular Dynamics Simulation of Longitudinal Space-Charge Induced Optical Microbunching

A. Marinelli, J. B. Rosenzweig and A. Pham
UCLA Dept. of Physics and Astronomy

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The Problem

- Observed coherent *optical* transition radiation (COTR) from FEL injector beams
- Some structure formation in beam at microscopic (<$\mu$m) level; near the mean inter-particle distance. How?
- Phenomenon related to transversal of dispersive sections
- Longitudinal and transverse spectra show stochastic behavior, 3D effects
Boundary Cond’ns: observations

- Data from LCLS, DESY FLASH, ANL, etc…
- No COTR upstream of bends
- Large enhancement possible after 1st bends
Spectral information constrains micobunching models: FLASH example

- High resolution COTR exp’ts reported
  - Multi-spike spectra
  - Transverse imaging indicates not simple 1D bunching

Figure 7: Selection of transverse profiles at different on-crest configurations and various spectral filters. The dimensions of the images are $2 \times 2 \text{ mm}^2$

Schmidt, et al., FEL 2009 (WEPC50)

Figure 7: Single shot (dots) and averaged (line) CTR spectrum between 0.95 $\mu$m and 1.7 $\mu$m measured with a commercial InGaAs spectrograph. The response of the detector is basically flat between 1.0 $\mu$m and 1.7 $\mu$m.
Interesting limit for beam organization: crystalline beams

- Emittance dominated beam: gas
- Space-charge dominated beam: liquid
- Coulomb (Wigner) crystal: solid
- Density $n = \lambda^{-3}$
- Compare ratio of
  - Potential energy $qV \propto e^2 / \lambda = e^2 n^{-1/3}$
  - Kinetic energy $k_B T \propto m_e \omega_p^2 \delta x^2$
- Crystal formed when $\Gamma = qV / k_B T \propto (\lambda / \delta x)^2 >> 1$
- Evaluate in rest frame $\Gamma = \frac{e^2 n_b^{1/3}}{k_B T}$
Can we have 1D crystal conditions in photoinjector?

- Transverse focusing gives higher temperatures $\Gamma$ small and time dependent conditions
  - No transverse crystallization possible
- Longitudinal 1D crystal OK
  - Observed in storage rings
  - Schottky spectral signature: noise suppression, spectral spikes near crystal $\lambda$
  - Still have $\Gamma$ too small at linac entrance
    - Overtaking of particles in $\zeta$ possible
  - Acceleration produces rapid cooling
    - In lab frame, $k_B T_z=2$ keV, but at LCLS linac exit, rest frame $k_B T_z=8$ eV...
    - In lab frame: “freezing” of longitudinal motion
    - At linac exit $\lambda \sim 800$ nm, rest frame $\Gamma \approx 300$
Analytical Models

THREE-DIMENSIONAL ANALYSIS OF LONGITUDINAL SPACE CHARGE MICROBUNCHING STARTING FROM SHOT NOISE

D. Ratner, A. Chao, Z. Huang
Stanford Linear Accelerator Center, Stanford, CA 94309, USA

“Collective-Interaction Control and Reduction of Optical Frequency Shot Noise in Charged-Particle Beams”
A. Gover and E. Dyunin
Phys. Rev. Lett. 102, 154801 (2009)

Quasicrystalline Beam Formation in RF Photoinjectors

Molecular dynamics simulations

- Resolution well below $\lambda$ needed
- Like to have full beam 3D geometry
  - Computationally intensive
- “Rest frame” quasi-electrostatic analysis
  - Transverse, longitudinal focusing
  - Macro-space-charge defocusing
  - Longitudinal “stretching” due to acceleration
  - Fourier approach to $\mu$-scopic fields
- 1st pass: use deformable box for beam center
  1E4 electrons, widths 10-50$\lambda$

Simulation box follows macro-envelope dynamics
Periodicity in 3D for High Resolution Simulations

We are interested in simulating only a fraction of the beam to obtain high resolution.

To enforce the right shot-noise statistics and particle to particle coulomb interaction, each particle is associated with a single electron.

An unphysical outward pressure would cause the beam to expand if only a small fraction of the beam was included.
Periodicity in 3D for High Resolution Simulations

By imposing periodicity in 3D we avoid beam expansion in transverse dimension. Electrons behave as if they were in the center of the beam!

Periodicity arises naturally using Fourier methods for space-charge force calculation.

Field calculated in the rest frame and then Lorentz-transformed back to the Lab Frame.

\[ \rho (\vec{x}) \xrightarrow{\text{FFT}} \tilde{\rho} (\vec{k}) \xrightarrow{} \tilde{E}(\vec{k}) = \frac{i\vec{k} \tilde{\rho} (\vec{k})}{k^2} \xrightarrow{\text{IFFT}} \tilde{E} (\vec{x}) \]
Periodic field solver using standard Fourier methods

Example: $E_y$ as a function of $x$ and $z$
Macroscopic Motion

X and Y sides of the box evolve through the macroscopic envelope equation leaving the ratio of boxSize/$\sigma_x$ constant:

$$\sigma''(\xi, z) + \left( \frac{\gamma'(\xi)}{\gamma(z)} \right) \sigma'(\xi, z) + \frac{\eta}{8} \left( \frac{\gamma'(\xi)}{\gamma(z)} \right)^2 \sigma(\xi, z) = \frac{r_e \lambda(\xi)}{\gamma(z)^3 \sigma(\xi, z)}$$

Head and tail of the box follow equations of motion in RF bucket.

Solenoid and RF focusing, acceleration as well as macroscopic beam self-force are also included in the equations of motion of the particles.
Range of Applicability

- Restriction to a small fraction of the beam requires quasi-laminar flow (no transverse mixing).

- Periodicity requires observation of wavelengths in the rest-frame smaller than the longitudinal and transverse sizes of the beam. (full-filled for optical and sub-optical microbunching).
Example: SPARC-like (LCLS with solenoid focusing)

Simulation parameters:

- InC, 100 Amps beam,
- Invariant envelope propagation
- No initial energy spread.
- 4000 particles
- 128 x 128 x 512 grid points (260 gridpoints/particle!)
Longitudinal Phase Space After 150 MeV Acceleration
Trace Space Before and After R56

Optical Microbunching!
LCLS-Like Case, Microbunching After BC1 for the 250 pC Beam
Application of code to noise reduction?

- The results are in good agreement with the theory for the value of the plasma oscillation period.
- Some macroscopic 3D effects are missing (suppression of collective behaviours at short wavelengths should limit the shot-noise reduction. At optical wavelengths. Abusing starting assumptions for periodicity?).

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“Collective-Interaction Control and Reduction of Optical Frequency Shot Noise in Charged-Particle Beams”
Code limitations and extension

- Periodic boundary conditions limit transverse beam structure resolution to box-size
- Need to understand transverse structure
  - Also in COTR data (virtual photon analysis)
- Extend to full beam size transversely
  - Large memory demand for particles
  - Use Hermite-Gaussian mode analysis for fields
  - Implement soon